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Specialisation in Systems, Analysis and Computational Sciences

Master's thesis

# Canonical Dirac structure of unitary quantum dynamics

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**Abstract**

We identify a unique system theoretic additive decomposition of any materially composite quantum system in terms of independent subsystems with probability ports and their interconnection through a Dirac structure. Conversely, we provide a terminating algorithm to determine the admissibility of additive compositions if the resulting quantum system is required to consist of elementary particles.

# Contents

# 1 Introduction

This thesis identifies a universally applicable decomposition of the unitary dynamics of quantum systems in terms of additive subsystems interconnected by a Dirac structure through probability ports.

The resulting formalism affords a system theoretic treatment of quantum mechanics that operationally resembles what port-Hamiltonian theory [vdSJ14; DMSB09] achieves for classical systems. However, the entirely different conceptual framework required by quantum theory in order to describe physical reality makes it necessary to rethink the composition and recomposition of systems from first principles as laid down by the postulates of quantum mechanics. Our careful phrasing of these postulates in Section 2 mathematically defines quantum theory and will provide the assumptions from which all results will be derived.

Only the final results will then resemble structures and ways of thinking known from port-Hamiltonian theory. Most remarkably, Dirac structures [DvdS98] will play precisely the same role in quantum mechanics. But already the ports, which give port-Hamiltonian theory its name [vM95], do not negotiate the transfer of energy between subsystems, but the transfer of probability instead. In this sense, we find a port-probability theory for quantum mechanics, which indeed requires and allows one to pose and answer qualitatively very different questions than one would and could ask in port-Hamiltonian theory.

Despite the need to go into quite subtle detail about the structure of quantum systems in the technical chapters to follow, it is possible to provide a rather precise mathematical sketch of how the results of this thesis build on the basic dynamical equation of quantum mechanics and how the latter is rewritten in terms of the formalism we develop. We now turn to this basic exposition.

It is well known that as long as no measurement takes place, the evolution of an observer's maximal knowledge (see Section 3) [SN20]

$$\rho = \frac{\langle\psi|\cdot\rangle\psi}{\langle\psi|\psi\rangle} \tag{1.1}$$

about the state of a quantum system is described by Schrödinger's ordinary differential equation[SN20]

$$\dot{\psi} = -iH\psi\,, \tag{1.2}$$

where $H$ is a self-adjoint operator with positive spectrum on a separable complex Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ and $\psi$ is a differentiable curve in the domain of $H$.

In order to keep any technical complexity that is inessential to the results obtained in this thesis at a minimum, we will consider quantum systems without translational degrees of freedom only. We will show that the Hilbert space is then finite-dimensional and all operators are bounded and thus defined everywhere.

The original seed for the research reported in this thesis is the seemingly trivial rewriting of equation (1.2) as

$$(\psi, \dot{\psi}) \in \mathcal{D}\,, \tag{1.3}$$

where

$$\mathcal{D} := \{(e, f) \in \mathcal{H} \times \mathcal{H} \mid f = -iHe\}\,. \tag{1.4}$$

What makes this interesting is the fact that the subset $\mathcal{D} \subset \mathcal{H} \times \mathcal{H}$ is a so-called Dirac structure [DMSB09] with respect to a pairing provided by the real-valued and merely $\mathbb{R}$-bilinear inner product

$$\langle\cdot|\cdot\rangle_{\mathcal{D}} : \mathcal{H} \times \mathcal{H} \to \mathbb{R}\,, \quad \langle\alpha|\beta\rangle_{\mathcal{D}} := 2\,\mathrm{Re}\,\langle\alpha|\beta\rangle \tag{1.5}$$

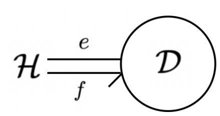
that is induced by the hermitian inner product $\langle\cdot|\cdot\rangle$.

Indeed, the first of two conditions to be satisfied by a Dirac structure is that every one of its elements $(e, f)$ makes the pairing $\langle e|f\rangle_{\mathcal{D}}$ vanish. This is easily established for our $\mathcal{D}$, since

$$\langle e|f\rangle_{\mathcal{D}} = \langle e| - iHe\rangle_{\mathcal{D}} = 2\,\mathrm{Re}(-i\langle\psi|H\psi\rangle) = 0 \tag{1.6}$$

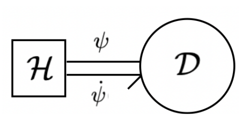
due to the hermiticity of $H$. The second condition is that the dimension of the Dirac structure is half the dimension of the space it is embedded in. For the case of our $\mathcal{D}$, this amounts to the condition that $\dim\mathcal{D} = \dim\mathcal{H}$, which however immediately follows from the positive spectrum and the resulting invertibility of $H$.

It is convenient to represent the above Dirac structure $\mathcal{D}$ diagrammatically as




where the double line represents the pair $(e, f)$ with $f$ being denoted next to the line that carries the half-arrow tip. The pair $(e, f)$ represents a so-called port of the Dirac structure [vM95] and $\mathcal{H} \times \mathcal{H}$ is the so-called port space. This terminology will be further refined below.

The Dirac structure is a purely algebraic object and is to be carefully distinguished from the differential equation $(\psi, \dot{\psi}) \in \mathcal{D}$ it governs. The latter is diagrammatically represented as



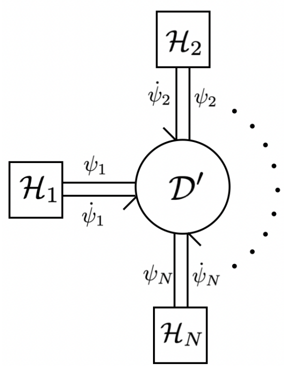

and involves a differentiable curve $\psi$ in the Hilbert space $\mathcal{H}$.

**Research Question 1**

The first research problem posed and solved in this thesis is how any quantum systems with Hilbert space $\mathcal{H}$ can be additively decomposed as

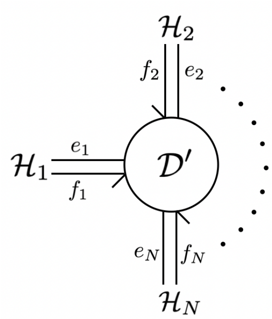
$$\mathcal{H} = \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_N$$

into a finite number of well-defined subsystems with uniquely determined Hilbert spaces such that the the equations of motion can be rewritten such as to correspond to a more refined diagram




that employs a refined Dirac structure $\mathcal{D}' \subset \mathcal{H}_1 \times \mathcal{H}_1 \times \mathcal{H}_2 \times \mathcal{H}_2 \times \cdots \times \mathcal{H}_N \times \mathcal{H}_N$ with respect to a suitable pairing $\langle \cdot | \cdot \rangle_{\mathcal{D}'}$. The additivity of the composition is required in order to allow for later replacement of any individual subsystem in favour of another, typically more sophisticatedly modelled one. This will be explained in more detail below.

Note that the underlying Dirac structure




now posseses $N$ ports associated with port spaces $\mathcal{H}_1 \times \mathcal{H}_1$ through to $\mathcal{H}_N \times \mathcal{H}_N$.

The diagrammatical simplicity, in which this first problem is phrased, hides the significant conceptual hurdles to be cleared in order to make this work in the context of quantum theory.

One key challenge is that the postulates of quantum mechanics [NC10; vNeu55] decidedly assert that $M$ quantum systems with Hilbert spaces $\mathcal{H}'_1, \ldots, \mathcal{H}'_M$ correspond to one total quantum system with Hilbert space

$$\mathcal{H} = \mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_M ,$$

and thus, generically,

$$\mathcal{H} \neq \mathcal{H}'_1 \oplus \cdots \oplus \mathcal{H}'_M .$$

The only way out of this dilemma is the realisation that the individual subsystems of the desired direct sum decomposition cannot be quantum systems in the sense of the postulates of quantum mechanics, but must be chosen such as to be commensurate with the tensor product construction.

The challenge thus becomes to study whether the postulates of quantum mechanics provide a unique additive decomposition for each system that is composed according to the tensorial composition rule of quantum mechanics, such that

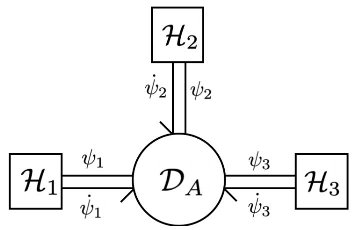
$$\mathcal{H}'_1 \otimes \cdots \otimes \mathcal{H}'_M = \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_N . \tag{1.7}$$

This is indeed achieved in Section 4 by careful consideration of the role of the isometry group of the physical space in which the quantum systems of interest are embedded. The solution to this key problem requires a deep result from representation theory that relates projective representations of a Lie group to linear representations of the universal covering group of that Lie group [Bar54] in order to then employ standard representation theory[Geo99] to then realise that (1.7) is to be understood as an equality of representation spaces rather than mere vector spaces.

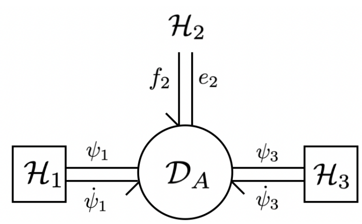
Another key challenge is to identify, the Dirac structure $\mathcal{D}'$ that interconnects the by then uniquely identified set of additive subsystems for any given quantum system. The obvious first step is a rewriting of the evolution equation (1.2) in terms of a set of $N$ subsystem equations, one for each of the additive subsystem Hilbert space $\mathcal{H}_1, \ldots, \mathcal{H}_N$ that have been identified uniquely, in input-output form. The challenge to be overcome here is that these equations seem to require that $\mathcal{D}'$ feature $N$ ports, each of which with port space $(\mathcal{H} \times \mathcal{H})$. This does not satisfy our diagrammatically stated aim of $\mathcal{D}'$ featuring $N$ ports with respective port spaces $\mathcal{H}_1 \times \mathcal{H}_1$ through to $\mathcal{H}_N \times \mathcal{H}_N$, which are much smaller and do not depend on the presence of any one of the other ports. This challenge is solved by exploitation of the fundmantally asserted linearity of the unitary evolution equation, which allows to shift the data contained in the energy operator $H$ quite freely into various Dirac substructures such as to obtain the desired decomposition of the equations of motion for the entire system. This is achieved in several steps in Section 5.

At this stage, the formalism now allows to convert previously closed quantum mechanical systems into open subsystems that can be additively composed with other such systems.

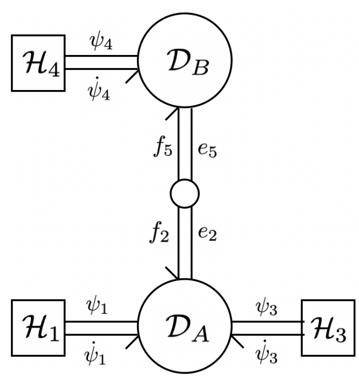
Consider, for instance, a quantum system whose additive decomposition yields the closed system of equations




Unplugging the second subsystem, one obtains the underdetermined (open) system of equations $(\psi_1, \dot\psi_1, e_2, f_2, \psi_3, \dot\psi_3) \in \mathcal{D}_A$ with the diagrammatic representation




where $(e_2, f_2)$ denotes now a so-called free port. This is interesting, since one may now connect another subsystem with an open port that features the same port space to obtain a another closed system such as, for example,




The connection diagrammatically represented by a small circle here is afforded by the algebraic equations [DMSB09]

$$f_5 = -f_2 \qquad \text{and} \qquad e_5 = e_2\,. \tag{1.8}$$

Indeed, it is straightforward to establish that the thus defined composition of the two Dirac structures $\mathcal{D}_A$ and $\mathcal{D}_B$ yields again a Dirac structure [vdSJ14].

Thus the resulting system is again a closed quantum system. The advantage from a modelling perspective is clear: One may refine or coarsen the modelling of any open subsystem by replacing it with another subsystem. The detailed construction in Section 5 will further reveal the pairing $\langle e|f\rangle$ obtained from any one port $(e, f)$ to encode the probabilty flow through that port. The half-arrow in the diagrammatic representation of a port is chosen such as to point towards the structure to which probability flows if $\langle e|f\rangle$ is positive.

**Research Question 2**

The second research question that can be asked and answered now, on the strength of the previously obtained results, is: Which open systems can be composed such as to produce a quantum system that can be thought of as being composed of elementary particles only?

The challenge posed by this question is now conceptually simple, since a quantum system is said to be composed of elementary particles if and only if its total Hilbert space is a tensor product

$$\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_M$$

of *irreducible* representation spaces of the underlying universal covering group of the isometry group of the physical space.

For quantum systems without translational degrees of freedom in Euclidean three-space, the second research question thus condenses to the following technical problem: For which positive integer $N > 1$, non-negative integers $a_1, \ldots, a_N$ and non-negative half-integers $j_1, \ldots, j_N$ does the direct sum of (without loss of generality: irreducible) representation spaces

$$a_1\mathbb{C}^{2j_1+1} \oplus \cdots \oplus a_N\mathbb{C}^{2j_N+1} \tag{1.9}$$

combine into a tensor product

$$\mathbb{C}^{2k_1+1} \otimes \cdots \otimes \mathbb{C}^{2k_M+1}$$

of irreducible representation spaces for a suitable integer $M > 1$ and suitable non-negative half-integers $k_1, \ldots, k_M$.

We provide a complete answer in form of a terminating algorithm in Section 6.

Section 7 concludes with a summary and outlook.

# 2 Postulates of quantum mechanics

In order to lay the foundations for the work that follows, we carefully formulate the postulates of quantum mechanics. From the mathematical point of view, these postulates amount to definitions of the terms quantum system, (knowledge of an observer about the) state of a quantum system and measurement apparatus.

## 2.1 Embedding of a quantum system in physical space

On the coarsest level, a mathematical model of any quantum system situated in some physical space starts with a Hilbert space.

**Postulate 1.** The mathematical description of a physical quantum system is built on a triple

$$(\mathcal{H}, \langle\cdot|\cdot\rangle, R) \tag{2.1}$$

consisting of a separable complex Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ that arises as the representation space of a projective unitary representation $R : G \to U(\mathcal{H})/\mathbb{C}^*$ of the isometry group $G$ of the mathematical model of the physical space in which the quantum system is situated.

*Remark* 1.1. In non-relativistic theory, the standard model for physical space is Euclidean three-space, whose isometry group $G$ is the special Euclidean group $SE(3) = T(3) \rtimes SO(3)$, i.e., the semi-direct product of the translation group and the rotation group in three dimensions[AVW13].

*Remark* 1.2. Infinite-dimensional Hilbert spaces arise for quantum systems with non-compact isometry groups only[Wey27]. Since the treatment of infinite-dimensional Hilbert spaces introduces formidable technical subtlety without introducing qualitatively new features in the related quantum theory, we restrict attention to quantum systems described by finite-dimensional Hilbert spaces. For non-relativistic theory, this restriction corresponds to disregarding the non-compact normal subgroup $T(3)$ of $SE(3)$, leaving one with the compact isometry group $SE(3)/T(3) = SO(3)$.

*Remark* 1.3. Projective representations $R$ are technically cumbersome to study and use. Fortunately, a weak technical condition on the isometry group $G$ of the ambient physical space (namely that its second Lie algebra cohomology is trivial) allows us to consider, in their stead, linear representations $\overline{R}$ of the universal covering group $\overline{G}$ of the isometry group. This is Bargmann's theorem and applies, in particular, to the special Euclidean group $SE(3)$ that underlies the setting studied in this thesis[Bar54].

*Remark* 1.4. There is typically more than one, and often infinitely many, different projective unitary representations of a given isometry group (or, linear representations of the universal covering group of the isometry group)[Geo99]. These different Hilbert spaces correspond to different quantum systems that can exist, from a theoretical point of view, in the given physical space. Hence, finding all representations of a given isometry group amounts to a classification of all possible quantum systems in a given physical space.

We emphasize again that, from now on, we only consider the quantum systems with finite-dimensional Hilbert spaces. This technically greatly simplifies the statement of all further postulates.

## 2.2 Material composition of quantum systems

If two or more quantum systems are situated in the same physical space, they cannot be described independently of each other. In fact, one cannot understand the total system in terms of the constituent physical systems.

**Postulate 2.** Two physically distinguishable quantum systems that are present in the same physical space with isometry group $G$ must be treated as one total quantum system in that physical space. If the description of the two constituent systems is built on the triples $(\mathcal{H}_1, \langle\cdot|\cdot\rangle_1, R_1)$ and $(\mathcal{H}_2, \langle\cdot|\cdot\rangle_2, R_2)$ then the total system is built on the triple $(\mathcal{H}, \langle\cdot|\cdot\rangle, R)$ where

$$\mathcal{H} \coloneqq \mathcal{H}_1 \otimes \mathcal{H}_2 \tag{2.2}$$

is the tensor product of vector spaces equipped with the inner product $\langle\cdot|\cdot\rangle$ determined by linear continuation of

$$\langle \alpha_1 \otimes \alpha_2 \mid \beta_1 \otimes \beta_2 \rangle \coloneqq \langle \alpha_1 \mid \beta_1 \rangle_1 \langle \alpha_2 \mid \beta_2 \rangle_2 \tag{2.3}$$

for any $\alpha_1, \beta_1 \in \mathcal{H}_1$ and $\alpha_2, \beta_2 \in \mathcal{H}_2$ and the representation $R$ is determined for any $g \in G$ by linear continuation of

$$R(g)(\alpha_1 \otimes \alpha_2) \coloneqq R_1(g)(\alpha) \otimes R_2(g)(\beta) \tag{2.4}$$

for any $\alpha_1 \in \mathcal{H}_1$ and $\alpha_2 \in \mathcal{H}_2$.

*Remark* 2.1. The above tensor product construction implies that the total quantum system cannot be understood by considering each of its constituent quantum systems separately. This explains why one must, rather than merely can, consider any two quantum systems in the same physical space as one total system.

*Remark* 2.2. The construction straightforwardly extends to any finite number of constituent quantum systems.

*Remark* 2.3. A representation is called irreducible if there is no non-trivial invariant subspace of the representation space[Geo99]. Irreducible representations correspond to elementary particles, since they cannot arise as tensor products of (non-trivial) representations. Conversely, the representation underlying any quantum systems that is ultimately composed of elementary particles must arise as a (multiple) tensor product of irreducible representations only. In this thesis, we assume that every quantum system is built of elementary particles. In other words, we only consider Hilbert spaces that arises as a (multiple) tensor product of irreducible representations.

*Remark* 2.4. For physically indistinguishable systems, all tensor products between spaces, vectors and representations are to be replaced by either symmetric tensor products (for particles with bosonic statistics) or anti-symmetric tensor products (for particles with fermionic statistics)[SN20]. In this thesis, we focus only on the composition of physically distinguishable quantum systems, since the adaptation to indistinguishable ones then follows.

## 2.3 Knowledge about the state of a quantum system

Quantum mechanics describes an observer's knowledge about the state of a quantum system. The remaining postulates all describe how an observer gains knowledge about a system and how that knowledge changes in time.

**Postulate 3.** An observer's knowledge about the state of a quantum system $(\mathcal{H}, \langle\cdot|\cdot\rangle, R)$ at some given time is mathematically represented by a positive unit trace operator on $\mathcal{H}$.
The temporal evolution of an observer's knowledge about the state of a quantum system is mathematically represented by a right-continuous *curve* $\rho$ in the space of all positive operators with unit trace.

*Remark* 3.1. Quantum mechanics is not a theory about the state of a quantum system, but only about an observer's knowledge about it. This is often hidden by the standard terminology that criminally shortens 'an observer's knowledge about the state of the quantum system' to 'the state of the quantum system' [SN20; Gri05].

*Remark* 3.2. There are two mutually exclusive mechanisms that determine the evolution of an observer's knowledge about the state of a quantum system: projective evolution at precisely those points in time when a measurement is performed and the observer takes notice of the measurement result (see postulate 6), and unitary evolution during time intervals where no measurement is made (see Postulate 7).

## 2.4 Measurement apparatuses

Observer can only gain knowledge about a quantum system by performing actual measurements on the system. One therefor first needs to provide a mathematical description of a measurement apparatus.

**Postulate 4.** An apparatus that can be used to perform a measurement on a given quantum system $(\mathcal{H}, \langle\cdot|\cdot\rangle, R)$ at an isolated point in time $t_{obs}$ is mathematically represented by a hermitian operator $M$ on $\mathcal{H}$. The elements of $\operatorname{spec}(M)$ are the only possible results the measurement apparatus can show.

*Remark* 4.1. Unless two measurements can be combined such as to constitute one single measurement described by one single hermitian operator, they cannot be performed at the same time.

*Remark* 4.2. The hermitian operator $M$ corresponding to the measurement apparatus is just an efficient way to capture all the mathematical data that characterize the apparatus. In turn, these data can be extracted from $M$ by the spectral theorem, which asserts that

$$M = \sum_{m \in \mathrm{spec}(M)} m P_m \,, \tag{2.5}$$

where $P_m$ is the unique orthogonal (hence hermitian) projector from $\mathcal{H}$ to the eigenspace $\mathrm{Eig}_m(M)$ and

$$\sum_{m \in \mathrm{spec}(M)} P_m = \mathrm{id}_{\mathcal{H}} \quad \text{and} \quad P_m P_n = \begin{cases} P_m \,, & m = n \\ 0 \,, & m \neq n \end{cases} \,. \tag{2.6}$$

The physical meaning of the projectors is clarified by the following two axioms.

## 2.5 Probabilistic prediction of measurement results

An observer knows the measurement outcomes that can result if a measurement is performed, but immediately until after the measurement, he or she can predict only the probability of a certain measurement outcome.

**Postulate 5.** An observer's knowledge about the state of a quantum system at a given point $t_{obs}$ in time does not suffice to predict which measurement result $m \in \mathrm{spec}(M)$ would be shown by a given measurement apparatus $M$ if the measurement is actually conducted. All an observer can predict, from his knowledge about the state and the measurement apparatus but without actually performing the measurement, is the probability

$$p(m|\rho(t_{obs})) := \mathrm{tr}(P_m^\dagger \rho(t_{obs}) P_m) \tag{2.7}$$

for the measurement apparatus to show the measurement result $m$.

*Remark* 5.1. Note that $P_m^\dagger \rho(t_{obs}) P_m$ is the projection of the operator $\rho(t_{obs})$ to the subspace of $\mathcal{H}$ that is given by the range of $P_m$.

## 2.6 Update of knowledge after read-off measurement

An observer's knowledge about the system is different depending on whether the observer reads-off the measurement result after the measurement has occurred. This can be a voluntary or involuntary decision.

**Postulate 6.** When an actual physical measurement is performed at time $t_{obs}$, the measurement apparatus shows precisely one of the elements of spec$(M)$ as the measurement result. In case an observer reads off this measurement result, his knowledge about the state of the system a time $t_{obs}$ is updated to

$$\rho(t_{obs}) := \frac{P^\dagger_{m_{obs}} \rho_{\text{prior}} P_{m_{obs}}}{\text{tr}(P^\dagger_{m_{obs}} \rho_{\text{prior}} P_{m_{obs}})}\,, \tag{2.8}$$

where $\rho_{\text{prior}} := \lim_{t \to t^-_{obs}} \rho(t)$ is the observer's knowledge about the state of the quantum system right before the measurement.

*Remark* 6.1. A measurement at $t_{obs}$, as described by Postulate 6, extends the previous temporal evolution for all $t < t_{obs}$ to a right-continuous (but generically left-discontinuous) curve for all $t \leq t_{obs}$.

*Remark* 6.2. The generic discontinuity at $t_{obs}$ is often referred to as 'state collapse', but would much more aptly be termed 'gain of knowledge about the state of the quantum system'.

*Remark* 6.3. In case an observer learns than an actual measurement has been performed, but voluntarily or involuntarily does *not* read off the measurement result shown by the measurement apparatus, his gain of knowledge is reduced by the need to invoke the probabilities for each possible measurement result according to Postulate 5, in order to build the weighted sum of all possible knowledge updates according to Postulate 6. His or her knowledge about the system at time $t_{obs}$ is thus reset to

$$\rho(t_{obs}) := \sum_{m \in \text{spec}(M)} P^\dagger_m \rho(t_{obs}) P_m\,. \tag{2.9}$$

Note that another observer, who did read off the measurement result from the measurement apparatus, concludes that $\rho(t_{obs})$ after measurement is as in Postulate 6. This is only possible if, indeed, $\rho(t_{obs})$ describes a particular observer's knowledge of the state, rather than the state of the quantum system itself, cf. Remark 3.1.

## 2.7 Evolution of knowledge without measurement

The temporal evolution of an observer's knowledge during the time period in which no measurement takes place is deterministic.

**Postulate 7.** There is some hermitian operator $H$ that governs the evolution of an observer's knowledge about the state of a quantum system over time intervals between any two consecutive measurements at times $t_{obs_1}$ and $t_{abs_2}$. For any $t \in (t_{obs_1}, t_{obs_2})$, the evolution of an observer's knowledge is given by

$$\rho(t) = \exp\left(-iH(t - t_{obs_1})\right) \rho(t_{obs_1}) \exp\left(iH(t - t_{obs_1})\right). \tag{2.10}$$

*Remark* 7.1. The hermitian operator $H$ that governs the time evolution of an observer's knowledge between any two measurements is traditionally called the measurement operator for the energy of the system.

*Remark* 7.2. The unitary temporal evolution of an observer's knowlegde in the interval $(t_{obs_1}, t_{obs_2})$ described by Postulate 7 extends the previous temporal evolution for all $t \leq t_{obs_1}$ to a right-continuous curve for all $t < t_{obs_2}$.

*Remark* 7.3. Together, postulates 6 and 7 generate the entire temporal evolution of an observer's knowledge about the state of the quantum system, with one type of evolution alternatingly taking over from the other one.

# 3 Maximal and submaximal knowledge

It is conceptually and technically convenient to classify the knowledge about the state of a quantum system $(\mathcal{H}, \langle\cdot|\cdot\rangle, R)$ into two disjoint classes, namely maximal knowledge and submaximal knowledge.

## 3.1 Maximal knowledge

**Definition 3.1.** *An observer's knowledge $\rho$ about the state of a quantum system is called maximal if $\rho^2 = \rho$.*

Maximal knowledge about a quantum state can written in terms of a single (but not unique) element of the Hilbert space:

**Lemma 3.2.** *Let $\rho$ encode some maximal knowledge about the state of a quantum system. Then there exists a $\psi \in \mathcal{H}$ such that*

$$\rho = \frac{\langle \psi \mid \cdot \rangle}{\langle \psi \mid \psi \rangle} \psi \, . \tag{3.1}$$

*Proof.* By definition, $\rho$ is a projection. Indeed, it is an orthogonal projection since

$$\rho^\dagger(\mathrm{id}_\mathcal{H} - \rho) = \rho^\dagger - \rho^\dagger \rho = 0 \tag{3.2}$$

because $\rho$ is a positive operator and hence hermitian. But for orthogonal projections, $\mathrm{rank}(\rho) = \mathrm{tr}(\rho)$ and the trace condition thus yields $\mathrm{rank}(\rho) = 1$. But every one-dimensional projector can be written in the claimed form for some $\psi \in \mathcal{H}$. □

The next two lemmas show that maximal knowledge remains maximal under both unitary evolution (Postulate 7) and projective evolution (Postulate 6).

**Lemma 3.3.** *If the knowledge $\rho_{prior}$ of the system before a measurement, as described in Postulate 6, is maximal, then also the updated knowledge $\rho(t_{obs})$ after measurement is maximal.*

*Proof.* Suppose an observer's knowledge $\rho_{\mathrm{prior}}$ about a system immediately before measurement is maximal. Upon reading off a specific measurement value, the observer's knowledge is updated to

$$\rho(t_{obs}) = \frac{P^\dagger \rho_{prior} P}{\mathrm{tr}(P^\dagger \rho_{prior} P)} \, , \tag{3.3}$$

where $P$ is the projector associated with the read off measurement value. Hence

$$\mathrm{tr}(P^\dagger \rho_{prior} P) = \sum_i \langle \varepsilon_i \mid P^\dagger \rho_{prior} P \varepsilon_i \rangle = \frac{\langle P^\dagger \psi \mid P\psi \rangle}{\langle \psi \mid \psi \rangle} \, , \tag{3.4}$$

where $\varepsilon_1, \ldots, \varepsilon_{\dim \mathcal{H}}$ is an orthonormal basis and $\psi$ is a Hilbert space element that represents the maximal knowledge $\rho_{\text{prior}}$ according to Lemma 3.2. But then

$$\rho(t_{obs})(\alpha) = \frac{\langle P^\dagger \psi \mid \alpha \rangle}{\langle P^\dagger \psi \mid P\psi \rangle} P\psi \qquad \text{for all } \alpha \in \mathcal{H} \tag{3.5}$$

from which one finds immediately that

$$\rho(t_{obs})\big(\rho(t_{obs})(\alpha)\big) = \rho(t_{obs})(\alpha) \qquad \text{for all } \alpha \in \mathcal{H}\,, \tag{3.6}$$

which identifies the updated knowledge as maximal. □

**Lemma 3.4.** *If the knowledge $\rho(t_{obs})$ determined by a measurement apparatus at $t_{obs}$ is maximal, then $\rho(t)$ remains maximal for any $t > t_{obs}$ before the next measurement.*

*Proof.* Since the evolution of an observer's knowledge after a measurement at $t_{obs}$ is governed by

$$\rho(t) = U(t)\rho(t_{obs})U^\dagger(t)\,, \tag{3.7}$$

where $U(t) := \exp(-iH(t - t_{obs}))$ is unitary because the energy operator $H$ is hermitian, it immediately follows that $\rho(t)^2 = \rho(t)$ for all $t > t_{obs}$ until another measurement occurs. □

Lemmas 3.3 and 3.4 show that neither a read-off measurement nor the unitary temporal evolution between consecutive measurements alter the maximality of an observer's knowledge.

In other words, it is consistent to assume that an observer's knowledge is always maximal under the condition that all measurement results are read off by that observer. This is the position tacitly taken in virtually all introductions to quantum mechanics, where an observer's knowledge is encoded in a Hilbert space element $\psi \in \mathcal{H}$ rather than in a positive unit trace operator $\rho$ on $\mathcal{H}$.

## 3.2 Loss of maximal knowledge

An important condition for an observer's knowledge to stay maximal is that the observer reads off the results shown by all measurement apparatuses. However, if an observer voluntarily or involuntarily does not read off the measurement result, his or her update of knowledge must take into account all principally possible updates and necessarily weigh them according to their probability. In other words, the updated knowledge for such an observer is

$$\rho(t_{obs}) = \sum_{m \in \text{spec}(M)} p(m|\rho_{\text{prior}}) \frac{P_m^\dagger \rho_{prior} P_m}{\text{tr}(P_m^\dagger \rho_{prior} P_m)} = \sum_{m \in \text{spec}(M)} P_m^\dagger \rho_{prior} P_m\,, \tag{3.8}$$

which is indeed a positive operator since $\langle \alpha \mid P_m^\dagger \rho P_m \mid \alpha \rangle \geq 0$ for all $\alpha \in \mathcal{H}$ and for each $m \in \text{spec}(M)$ and its trace is one as the sum of all probabilities for the possible measurement outcomes. For such an observer, the updated knowledge may no longer be maximal.

## 3.3 Von Neumann's equation

Postulate 7 provides a curve $\rho$ in the space of positive unit trace operators that encodes the evolution of an observer's knowledge about the state of a quantum system while no measuremet occurs. This curve can be understood as the solution to an ordinary differential equation, which is known as von Neumann's equation and simply obtained by differentiation of equation (3.7),

$$\dot{\rho}(t) = -iHU(t)\rho(t_{obs})U^{\dagger}(t) + U(t)\rho(t_{obs})(-iHU(t))^{\dagger} = -i[H, \rho(t)]\,, \tag{3.9}$$

where the commutator $[A, B]$ between two operators $A$ and $B$ is defined as the operator $AB - BA$.

## 3.4 Schrödinger's equation

Von Neumann's equation simplifies for the special case when the evolution $\rho$ is maximal. It is then usually rewritten as an ordinary differential equation for a curve $\psi$ in Hilbert space that represents the observer's maximal knowledge through

$$\rho_{\psi}(t) := \frac{\langle \psi(t) \mid \cdot \rangle}{\langle \psi(t) \mid \psi(t) \rangle} \psi(t)\,. \tag{3.10}$$

Without loss of generality, one may choose a curve $\psi$ that is normalized, for if $\psi$ is not normalized, the curve $f\psi$ with

$$f(t) := \langle \psi(t) \mid \psi(t) \rangle^{-\frac{1}{2}} \tag{3.11}$$

is normalized and represents the same knowledge since $\rho_{f\psi} = \rho_{\psi}$. Insertion of $\rho_{\psi}$ for a normalized curve $\psi$ in Hilbert space, von Neumann's equation immediately reduces to

$$\langle \psi | \cdot \rangle (\dot{\psi} + iH\psi) + \langle \dot{\psi} + iH\psi | \cdot \rangle \psi = 0\,. \tag{3.12}$$

Thus von Neumann's equation for maximal knowledge is satisfied if the curve $\psi$ satisfies Schrödinger's equation

$$\dot{\psi}(t) = -iH\psi(t)\,. \tag{3.13}$$

# 4 Quantum systems in Euclidean three-space

In order to be able to employ linear, rather than projective representations in the study of quantum systems in Euclidean space, we identify the universal covering group of the special Euclidean group. We then immediately specialise to quantum systems without translational degrees of freedom, by dividing out the normal subgroup: the group of translations. This leaves us with the group of rotations as the isometry group of the physical space whose universal covering group is the special unitary group $SU(2)$. Its linear unitary representations and representations spaces underlie the mathematical description of any possible quantum system in Euclidean three-space without translation degrees of freedom.

## 4.1 Universal covering group of $SE(3)$

Physical space in non-relativistic theory is modelled by Euclidean three-space whose isometry group is the special Euclidean group [AVW13]

$$SE(3) = T(3) \rtimes SO(3) \;, \tag{4.1}$$

i.e., the semi-direct product of the group of translations $T(3)$, which is the normal subgroup of $SE(3)$ and the group of rotations $SO(3)$. Then, according to Postulate 1, the mathematical description of any quantum system situated in Euclidean-three space is underpinned by projective unitary representations and their representation spaces. Thus, one can determine all such quantum systems by classifying the projective unitary representations of $SE(3)$. This can, in turn, be accomplished by classifying all the linear representations of the universal covering group of $SE(3)$ instead. More precisely, $SE(3)$ satisfies the assumptions of Bargmann's theorem [Bar54] according to which, if the second Lie algebra cohomology group $H^2(\mathfrak{g}, \mathbb{R})$ of a connected Lie group $G$ with a Lie algebra $\mathfrak{g}$ is trivial, then every projective unitary representation $R$ of the Lie group $G$ on a Hilbert space $\mathcal{H}$ lifts to a linear unitary representation $\overline{R}$ of its universal covering group $\overline{G}$ on $\mathcal{H}$ such that the diagram

$$\begin{tikzcd} \overline{G} \arrow[r, "\overline{R}"] \arrow[d, "p"'] & U(\mathcal{H}) \arrow[d, "\pi"] \\ G \arrow[r, "R"] & U(\mathcal{H})/\mathbb{C}^* \end{tikzcd}$$

commutes, where $p$ is the universal covering map and $\pi$ is the canonical quotient map. The universal covering group $\overline{G}$ of a given Lie group $G$ is defined as the unique simply connected Lie group (meaning that the underlying manifold has trivial fundamental group) whose Lie algebra $\mathrm{Lie}(\overline{G})$ coincides with the Lie group $\mathrm{Lie}(G)$ [Geo99].

Since the group $SE(3)$ satisfies the assumptions of Bargmann's theorem, we study linear unitary representations of the universal covering group of $SE(3)$, which is

$$\overline{SE(3)} = \overline{T(3) \rtimes SO(3)} = \overline{T(3)} \rtimes \overline{SO(3)} = T(3) \rtimes SU(2)\,, \tag{4.2}$$

where the second equal sign holds because the universal cover distributes over the semi-direct product, because the fundamental group of a direct product of groups is the direct product of the respective fundamental groups and the fundamental group does not depend on the group operation that renders the direct product semi-direct. The universal covering group $\overline{T(3)}$ coincides with $T(3)$, whereas the universal covering group $\overline{SO(3)}$ is the special unitary group $SU(2)$.

## 4.2 Dividing out translational degrees of freedom

The irreducible linear unitary representations of $\overline{SE(3)}$ have as representation spaces the Hilbert spaces $L^2(\mathbb{R}^3) \otimes \mathbb{C}^d$ for all $d \in \mathbb{N}^*$[SN20]. However, since working with infinite-dimensional representations is filled with technical details that are irrelevant for the points we want to make, we will instead work with the quotient group $SE(3)/T(3) = SO(3)$. Physically, this means we are considering quantum systems in Euclidean three-space which have no translational degrees of freedom. The rotation group $SO(3)$ satisfies the assumptions of Bargmann's theorem by itself, which allows us to study linear unitary representations of $SU(2)$ instead. Since the group $SU(2)$ is compact, its irreducible unitary representations are, according to Peter-Weyl's theorem [Wey27], finite-dimensional. Hence, from the mathematical perspective, the description of a quantum system in Euclidean three-space without translational degrees of freedom falls in the scope of complex finite-dimensional linear algebra.

The same principles apply when transferring our study to physical spaces with a different isometry group, such as flat relativistic spacetime. The isometry group of the latter is the Poincaré group and dividing out translational degrees of freedom leads to the Lorentz group $SO(1,3)$, whose universal covering group is $SL(2,\mathbb{C})$[Geo99].

Unless stated otherwise, henceforth, quantum systems refers to quantum systems in Euclidean three-space without translational degrees of freedom.

## 4.3 Irreducible representations of $SU(2)$

We classify all quantum systems without translational degrees of freedom situated in Euclidean three-space by finding all linear unitary representations of $SU(2)$ and their respective representation spaces. Physically, this corresponds to determining all theoretically possible elementary particles, since they are, by definition, not reducible into more elementary constituents.

It is convenient to understand $SU(2)$ as a group of complex $2\times2$ unitary matrices of determinant one[Geo99]. Its Lie algebra can be generated by Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \ , \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ , \tag{4.3}$$

from which every element $g \in SU(2)$ (where the bar notation reminds us that this is an element of the universal covering group) can be obtained through

$$g = \exp\left(\tfrac{i}{2}\sum_{n=1}^{3}\alpha^n\sigma_n\right) \tag{4.4}$$

for some $\alpha^1, \alpha^2, \alpha^3 \in \mathbb{R}$.

One finds that all unitary representations of $SU(2)$ constitute a family whose members $\overline{R}_j : SU(2) \to U(\mathbb{C}^{2j+1})$ are labelled by a non-negative half-integer $j$ and are explicitly given by

$$\overline{R}_j\left(\exp\left(\tfrac{i}{2}\sum_{n=1}^{3}\alpha^n\sigma_n\right)\right) := \exp\left(\frac{i}{2}\sum_{n=1}^{3}\alpha^n J_n^j\right) \ , \tag{4.5}$$

where $J_n^j$ on the right hand side denotes the $n$-th generating matrix of the Lie algebra of the spin-$j$ representation. The entries in the $m$-th row and $m'$-th column of these generators are explicitly given by [Geo99]

$$\begin{aligned}
(J_1^j)^m{}_{m'} &:= \frac{1}{2}\left(\sqrt{(j-m)(j+m+1)\delta^m{}_{m'+1}} + \sqrt{(j+m)(j-m+1)\delta^m{}_{m'-1}}\right) \\
(J_2^j)^m{}_{m'} &:= \frac{1}{2i}\left(\sqrt{(j-m)(j+m+1)\delta^m{}_{m'+1}} - \sqrt{(j+m)(j-m+1)\delta^m{}_{m'-1}}\right) \\
(J_3^j)^m{}_{m'} &:= m\delta_{m,m'}
\end{aligned} \tag{4.6}$$

with $m$ and $m'$ ranging over $-j, -j+1, \ldots, j-1, j$.

The representation $\overline{R}_j$ is traditionally called the spin-$j$ representation. Note that the associated Hilbert space is $\mathbb{C}^{2j+1}$ equipped with its standard hermitian inner product. For our theoretical investigation, the identification of this representation space is the main result of this subsection. The explicit representation maps for the various spin-$j$ representations will, however, may be needed for some concrete calculations and are thus given here in detail.

## 4.4 $SU(2)$-invariant decomposition of tensor products

The tensor product $\overline{R}_{j_1} \otimes \overline{R}_{j_2}$ of two irreducible unitary representations $\overline{R}_{j_1}$ and $\overline{R}_{j_2}$ of $SU(2)$ gives rise to a reducible representation. One can show that any such representation is completely reducible. This means it can be written as a direct sum of finitely many irreducible unitary representations,

$$\overline{R}_{j_1} \otimes \overline{R}_{j_2} = \overline{R}_{|j_1-j_2|} \oplus \overline{R}_{|j_1-j_2|+1} \oplus \cdots \oplus \overline{R}_{j_2+j_2} \ , \tag{4.7}$$

where for any two linear unitary representations $\overline{R}_1 : G \to U(\mathcal{H}_1)$ and $\overline{R}_2 : G \to U(\mathcal{H}_2)$ the tensor product of representations is defined as the linear continuation of the map

$$\overline{R}_1 \otimes \overline{R}_2 : G \to U(\mathcal{H}_1 \otimes \mathcal{H}_2)\,, \quad (\overline{R}_1 \otimes \overline{R}_2)(g)(\alpha_1 \otimes \alpha_2) := \overline{R}_1(g)(\alpha_1) \otimes \overline{R}_2(\alpha_2) \tag{4.8}$$

while the direct sum of representations is given as the map

$$\overline{R}_1 \oplus \overline{R}_2 : G \to U(\mathcal{H}_1 \oplus \mathcal{H}_2)\,, \quad (\overline{R}_1 \oplus \overline{R}_2)(g)(\alpha_1 \oplus \alpha_2) := \overline{R}_1(g)(\alpha_1) \oplus \overline{R}_2(\alpha_2)\,. \tag{4.9}$$

The direct sum in 4.7, known as the Clebsch-Gordan decomposition [Geo99], is a unique $SU(2)$-invariant decomposition. In particular, this means that the representation space decomposes as

$$\mathbb{C}^{2j_1+1} \otimes \mathbb{C}^{2j_2+1} = \mathbb{C}^{2|j_1-j_2|+1} \oplus \mathbb{C}^{2(|j_1-j_2|+1)+1} \oplus \cdots \oplus \mathbb{C}^{2(j_1+j_2)+1} \tag{4.10}$$

and that the action of $(\overline{R}_{j_1} \otimes \overline{R}_{j_2})(g)$ on the left hand side corresponds to the action of $(\overline{R}_{|j_1-j_2|} \oplus \cdots \oplus \overline{R}_{j_1+j_2})(g)$ on the right hand side, which does not mix the various direct summand representation spaces. In other words, the above decomposition is unique and independent of the physical observer.

The subspaces that appear in the direct sum on the right hand side of (4.9) lie as follows in the tensor product space on the left hand side, namely such that

$$|M\rangle_J := \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C^{JM}_{j_1 j_2 m_1 m_2} |m_1\rangle_{j_1} \otimes |m_2\rangle_{j_2} \tag{4.11}$$

where, on the left hand side, the label $M = -J, -J+1, \ldots, J$ denotes the $M$-th basis vector of an orthonormal basis of the subspace $\mathbb{C}^{2J+1}$, while on the right hand side, the label $m_1 = -j_1, -j_1+1, \ldots, j_1$ and likewise for $m_2$ and $j_2$, while the $C^{JM}_{j_1 j_2 m_1 m_2}$ are the well-known Clebsch-Gordan coefficients for $SU(2)$ [Geo99].

The coefficients of the associated inverse transformation is given by the complex conjugates of the very same coefficients, due to the orthonormality of the involved bases. Adoption of the Condon-Shortley phase convention, however, renders all coefficients real [Geo99], so that, indeed,

$$|m_1\rangle_{j_1} \otimes |m_2\rangle_{j_2} = \sum_{J=|j_1-j_2|}^{j_1+j_2} \sum_{M=-J}^{J} C^{JM}_{j_1 j_2 m_1 m_2} |M\rangle_J\,. \tag{4.12}$$

There exists tables as well as recursive and closed formulae for the Clebsch-Gordan coefficients for $SU(2)$ with the said phase convention and we refer to those for concrete examples.

Knowledge of the existence of the above bijective correspondence between the induced basis for the tensor product and the induced basis for its Clebsch-Gordan direct sum decomposition suffices for the general theoretical developments of this thesis. The concrete coefficients are only needed for practical calculations.

Noting that a tensor product distributes over a direct sum,

$$\overline{R}_{j_a} \otimes (\overline{R}_{j_b} \oplus \overline{R}_{j_c}) = (\overline{R}_{j_a} \otimes \overline{R}_{j_b}) \oplus (\overline{R}_{j_a} \otimes \overline{R}_{j_c}) \ , \tag{4.13}$$

the decomposition (4.7) is straightforwardly applied also to the tensor product of finitely many representations of $SU(2)$.

# 5 Additive decomposition of closed systems

We are now in a position to show how the dynamics for an observer's maximal knowledge about any quantum system without translational degrees of freedom can be decomposed in terms of a Dirac structure and probability ports.

## 5.1 Schrödinger equation of a reducible quantum system

We consider the unitary dynamics of a quantum system $(\mathcal{H}, \langle\cdot|\cdot\rangle, \overline{R})$ whose underlying Hilbert space additively decomposes into the $SU(2)$ invariant decomposition of representation spaces of irreducible representations of $SU(2)$ as

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_N \tag{5.1}$$

and derive a set of $N$ equations, each with an input term that couples to all the other equations, as a first step in the overall construction of this section.

To each summand in the direct sum above we associate an orthogonal projection operator $P_n : \mathcal{H} \to \mathcal{H}_n \subset \mathcal{H}$ and

$$\sum_{n=1}^{N} P_n = \mathrm{id}_{\mathcal{H}} \quad \text{and} \quad P_m P_n = \begin{cases} P_n \, , & m = n \\ 0 \, , & m \neq n \end{cases} \, . \tag{5.2}$$

The Schrödinger equation

$$\dot{\psi}(t) = -iH\psi(t) \tag{5.3}$$

of a curve $\psi$ decomposes into $N$ coupled equations

$$\dot{\psi}_n(t) = -iP_n H P_n \psi_n(t) - iP_n H \sum_{\substack{k=1 \\ k\neq n}}^{N} P_k \psi_k(t) \, . \tag{5.4}$$

Each differential equation describes the unitary evolution of a subsystem which depends on the knowledge about its state $\psi_n(t) \coloneqq P_n\psi(t)$, but also on the knowledge about the states of all other subsystems. Thus, we introduce notation

$$H_{nn} \coloneqq P_n H P_n \, , \quad B_n \coloneqq -iP_n H(\mathrm{id}_H - P_n) \, , \quad u_{\overline{n}}(t) \coloneqq \psi(t) - \psi_n(t) \, , \tag{5.5}$$

in which the equations are of the form

$$\dot{\psi}_n(t) = -iH_{nn}\psi_n(t) + B_n u_n(t) \quad \text{for } n = 1, \ldots, N \, . \tag{5.6}$$

We call $B_n$ input matrix, and $u_n$ is called input, alluding to the input-output form in the systems theory.

## 5.2 Input-output formulation without ports

As a second step we now identify the $N$ output equations associated with the $N$ equations with input term found in the previous subsection. The most important conceptual result of this subsection, however, will be the emergence of an $\mathbb{R}$-bilinear pairing, which we will then refine in the following subsection.

The following construction uses the measurement postulates of quantum theory. In particular, we use that the probability for a measurement apparatus defined by an orthogonal projector $P_n$ (for any $n = 1, \ldots, N$) to yield the result 1 at time $t$ is

$$p(1|\rho(t)) = \mathrm{tr}(P_n \rho(t) P_n) = \frac{\langle \psi_n(t) \mid \psi_n(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} . \tag{5.7}$$

This is the probability to find an affirmative answer, from measurement, whether the system is described a state in $\mathcal{H}_n$. The probability flow $\dot{p}(1|\rho(t))$ as the system evolves is thus given by

$$\dot{p}(1|\rho(t)) = \frac{\langle \dot{\psi}_n(t) \mid \psi_n(t) \rangle + \langle \psi_n(t) \mid \dot{\psi}_n(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} = \frac{2\mathrm{Re}\langle \psi_n(t) \mid \dot{\psi}_n(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} , \tag{5.8}$$

where the first equality holds since the unitary time evolution for $\psi$ renders the derivative of its norm zero. We can now insert the input equation derived in the previous section into the right-hand side, and obtain

$$\frac{2\mathrm{Re}\langle \psi_n(t) \mid \dot{\psi}_n(t) \rangle}{\langle \psi(t) \mid \psi(t) \rangle} = \frac{2\mathrm{Re}\big(\langle \psi_n(t) \mid B_n u_n(t) \rangle\big)}{\langle \psi(t) \mid \psi(t) \rangle} . \tag{5.9}$$

Note that he term $-i\langle \psi_n(t) \mid H_{nn} \psi_n(t) \rangle$ is imaginary. Defining the output

$$y_n(t) := -B_n^\dagger \psi_n(t) , \tag{5.10}$$

we thus obtain from the above calculation the balance equation

$$2\mathrm{Re}\big(\langle \psi_n(t) \mid \dot{\psi}_n(t) \rangle\big) + 2\mathrm{Re}\big(\langle y_n(t) \mid u_{\overline{n}}(t) \rangle\big) = 0 . \tag{5.11}$$

Note that this balance equation requires use of the $\mathbb{R}$-bilinear real-valued pairing $2\,\mathrm{Re}\langle \cdot | \cdot \rangle$ defined on all of $\mathcal{H} \times \mathcal{H}$, whence the port space of a Dirac structure

$$\mathcal{D}'_n := \{(e_n, f_n, y_n, u_n) \in \mathcal{H}_n \times \mathcal{H}_n \times \mathcal{H}_{\overline{n}} \times \mathcal{H}_{\overline{n}} \mid f_n = -iH_{nn} e_n + B_n u_n \,, y_n = -B_n^\dagger e_n\} , \tag{5.12}$$

which one could in principle devise to describe the $n$-th subsystem equation as

$$(\psi_n, \dot{\psi}_n, y_n, u_n) \in \mathcal{D}'_n , \tag{5.13}$$

would use a port space $\mathcal{H}_{\overline{n}} \times \mathcal{H}_{\overline{n}}$ for its input and output to the environment that depends on the precisely which other subsystems are present. That is not desirable and will be repaired in the following subsection.

## 5.3 Input-output formulation with ports

The port of a subsystem must be independent of the presence of other subsystems that interconnect via a Dirac structure in order to allow for the simple star-shaped decompositions we are aiming for. Thus, despite superficial appearances, the input-output formulation arrived at above does not feature suitable ports, since the input and output of subsystem $\mathcal{H}_n$ are elements of $\mathcal{H}_{\overline{n}} = \bigoplus_{m \neq n} \mathcal{H}_m$ and thus completely dependent on which other subsystems are present.

As the third and last step to obtain a description of an additively decomposed quantum system in terms of ports and a Dirac structure, we now repair this shortcoming. This is done by describing the probability flow through a port of subsystem $\mathcal{H}_n$ exclusively through the pairing

$$\langle \cdot , \cdot \rangle_{\mathcal{D}_n} : \mathcal{H}_n \times \mathcal{H}_n \to \mathbb{R}\,, \quad \langle \alpha_n | \beta_n \rangle_{\mathcal{D}_n} := 2\,\mathrm{Re}\langle \alpha_n | \beta_n \rangle \tag{5.14}$$

which renders the subset

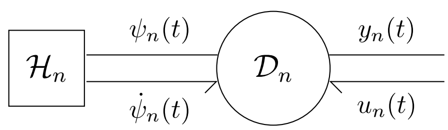
$$\mathcal{D}_n := \{(e_n, f_n, y_n, u_n) \in \mathcal{H}_n \times \mathcal{H}_n \times \mathcal{H}_n \times \mathcal{H}_n \mid f_n = -iH_{nn}e_n + u_n\,, y_n = -e_n\} \tag{5.15}$$

a Dirac structure.

While this now ensures that the ports of the $n$-th subsystem only depend on the Hilbert space for that subsystem, the equations of motion

$$(\psi_n(t), \dot{\psi}_n(t), u_n, y_n) \in \mathcal{D}_n$$

diagrammatically represented by




are no longer those of the input-output equations of the previous subsection, since they do not encode the information contained in the terms $B_n$. In the following subsection, we will show how one further Dirac structure will capture all that missing information.

## 5.4 Identification of interconnecting Dirac structure

We now interconnect the subsystems defined in the previous subsection such that the resulting equations of motion recover the unitary evolution of the maximal knowledge about the total quantum system.

To this end we define a Dirac structure

$$\mathcal{D}_{\mathrm{int}} \subset (\mathcal{H}_1 \times \mathcal{H}_1) \times (\mathcal{H}_2 \times \mathcal{H}_2) \times \cdots \times (\mathcal{H}_N \times \mathcal{H}_N)\,, \tag{5.16}$$

by the condition that $(z_1, v_1, \ldots, z_N, v_N) \in \mathcal{D}_{\mathrm{int}}$ if and only if

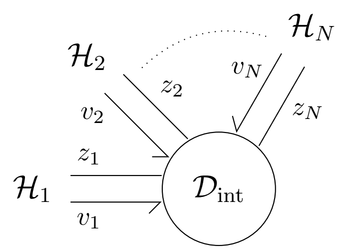
$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix} = -i \begin{pmatrix} 0 & H_{12} & H_{13} & \cdots & H_{1N} \\ H_{21} & 0 & H_{23} & \cdots & H_{2N} \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ H_{N1} & \cdots & \ldots & H_{N-1N} & 0 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_N \end{pmatrix}, \tag{5.17}$$

which we write more compactly as $v = -iBz$ in terms of the thus defined hermitian operator $B$ on $\mathcal{H}$. It is easily seen that $\mathcal{D}_{\text{int}}$ is indeed a Dirac structure since there are $N$ linear relations for $2N$ variables, so that $\dim(\mathcal{D}_{\text{int}}) = \dim \mathcal{H}$, and that the balance equation

$$\sum_{n=1}^{N} \langle z_n | v_n \rangle_{\mathcal{D}_n} = 2\mathrm{Re}(\langle z \mid -iBz \rangle) = 0 \, , \tag{5.18}$$

holds since $B^\dagger = B$ because $H_{ij}^\dagger = H_{ji}$.

It is now a simple exercise to show that the total system is reconstructed by composing the just identified Dirac structure



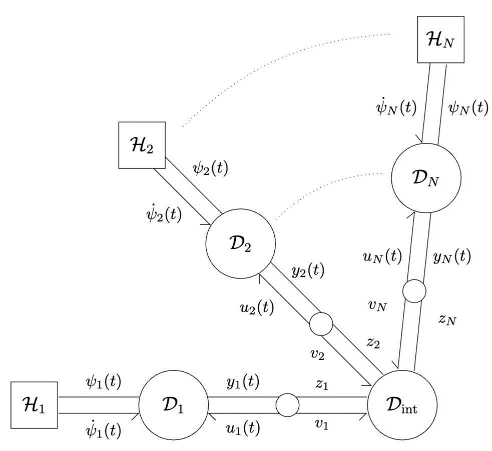

to the $N$ open subsystems defined in the previous subsection by virtue of $N$-fold application the previously encountered composition rule for Dirac structures,

$$u_n \coloneqq v_n \quad \text{and} \quad y_n \coloneqq -z_n \qquad \text{for } n = 1, \ldots, N \, , \tag{5.19}$$

which are diagrammatically represented by small circles that connect two ports with the same port space. The resulting equations of motion

$$(\psi_1, \dot{\psi}_1, \ldots, \psi_N, \dot{\psi}_N) \in \mathcal{D}_N \circ (\cdots \circ (\mathcal{D}_2 \circ (\mathcal{D}_1 \circ \mathcal{D}_{\text{int}}))) \cdots)$$

amount precisely to equation (5.3) and have the the diagrammatic representation



## 6 Additive composition of open systems

A question that can now be meaningfully formulated and answered is whether a quantum system given by an additive composition of subsystems as described in the previous section is, in fact, physically possible in the sense that it can be considered to be materially composed of only elementary particles? We provide a terminating algorithm to decide this question.

### 6.1 Admissible decompositions

We wish to understand for which positive integer $N > 1$, non-negative integers $a_1, \ldots, a_N$ and non-negative half-integers $j_1, \ldots, j_N$ does the direct sum of (without loss of generality: irreducible) representation spaces

$$a_1\mathbb{C}^{2j_1+1} \oplus \cdots \oplus a_N\mathbb{C}^{2j_N+1} \tag{6.1}$$

combine into a tensor product

$$\mathbb{C}^{2k_1+1} \otimes \cdots \otimes \mathbb{C}^{2k_M+1} \tag{6.2}$$

of irreducible representation spaces for a suitable integer $M > 1$ and suitable non-negative half-integers $k_1, \ldots, k_M$.

We call an additive decomposition admissible, if it corresponds to such a tensor product of irreducible representation spaces,

### 6.2 Unit multiplicities

We start by studying the additive decompositions that arise from a tensor product of two irreducible representations through a the Clebsch-Gordan decomposition (4.10), which we rewrite as

$$\mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2} = \bigoplus_{i=\frac{|n_1-n_2|}{2}}^{\frac{n_1+n_2}{2}-1} \mathbb{C}^{2i+1} \,. \tag{6.3}$$

We expressed $j_i$ in terms of $n_i = 2j_i + 1$ for $i = 1, 2$. We also assume, without loss of generality, that $n_1 \geq n_2$, in order to remove the absolute value in the subtraction. Since vector spaces in the decomposition differ only in their dimensions, we will write just the dimensions. By direct calculation, one obtains

$$n_1 \otimes n_2 = (n_1 - n_2 + 1) \oplus (n_1 - n_2 + 3) \oplus \cdots \oplus (n_1 + n_2 - 1) \,. \tag{6.4}$$

*Observation* 6.1. The multiplicity of each summand is one.

*Observation* 6.2. Since $n_1$ and $n_2$ are natural numbers, $n_1 \pm n_2$ can be either even or odd. More precisely,

(i) if both $n_1$ and $n_2$ have the same parity, then $n_1 \pm n_2$ is even, and the summands will be odd naturals in the range $[n_1 - n_2 + 1, n_1 + n_2 - 1]$,

(ii) if $n_1$ and $n_2$ are of opposite parities, then $n_1 \pm n_2$ is odd, and the summands are all even naturals in the range $[n_1 - n_2 + 1, n_1 + n_2 - 1]$.

*Observation* 6.3. The number of terms in the sum does not depend on $n_1$. The number of iterations of the sum is

$$\left(\frac{n_1 + n_2}{2} - 1\right) - \frac{n_1 - n_2}{2} = n_2 - 1 \; , \tag{6.5}$$

so there are $n_2$ terms in the sum.

*Conclusion* 6.1. If and only if all the summands in an additive decomposition are of unit multiplicity and their dimensions are either all the consecutive even or all the consecutive odd naturals within some finite range, then the additive decomposition represents a material composition of two particles whose Hilbert spaces have dimensions

$$n_1 = \frac{1}{k} \sum_i m_i \qquad \text{and} \qquad n_2 = k \; , \tag{6.6}$$

which are the average of the sum of all dimensions and the number of terms in the additive decomposition.

*Observation* 6.4. The numbers $n_1$ and $n_2$ are unique, so a conceptual decomposition can correspond to only one material decomposition.

*Example* 6.1. Consider an additive decomposition given as

$$\mathbb{C}^4 \oplus \mathbb{C}^6 \oplus \mathbb{C}^8 \oplus \mathbb{C}^{10}$$

Dimensions consist of all even naturals in the range $[4, 10]$. Since there are four terms, $n_2 = 4$. The average is seven, so $n_1 = 7$. One can check that indeed,

$$\mathbb{C}^7 \otimes \mathbb{C}^4 = \mathbb{C}^4 \oplus \mathbb{C}^6 \oplus \mathbb{C}^8 \oplus \mathbb{C}^{10} \; .$$

## 6.3 Multiplicities larger than one

With Observation 6.1 in mind, we know that if there is an $a_n > 1$ for some $n = 1, \dots, N$, we have to consider a material composition of more than two systems, i.e.,

$$\mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2} \otimes \cdots \otimes \mathbb{C}^{n_N} \; , \quad N > 2 \tag{6.7}$$

There is no closed-form expression for a Clebsch-Gordan decomposition of a multiple tensor product. Thus one must study such situations case-by-case. However, there are some properties one can check in order to determine whether a certain additive decomposition corresponds to a tensor product of irreducible representations.

*Observation* 6.5. The sum of dimensions $m = \sum_{i=1}^{k} a_i m_i$ of the additive composition must be a composite number with at least three non-trivial divisors. In general, there might be more ways one can factorize $m$, and the number of factors might vary.

*Observation* 6.6. As a consequence of Observation 6.2 and the distributivity of addition over a tensor product, the additive decomposition must consist of vector spaces whose dimensions are all the consecutive naturals of the same parity within some finite range, with a possible multiplicity that is larger than one. Consider the three-fold tensor product

$$(\mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2}) \otimes \mathbb{C}^{n_3} = \bigoplus_{i=\frac{n_1-n_2}{2}}^{\frac{n_1+n_2}{2}-1} \mathbb{C}^{2i+1} \otimes \mathbb{C}^{n_3} \,. \tag{6.8}$$

Since the dimensions $2i+1$ on the right-hand side all have the same parity, the summands resulting from the Clebsch-Gordan decomposition of each tensor product $\mathbb{C}^{2i+1} \otimes \mathbb{C}^{n_3}$ again have the same parity that depends only on the parity of $n_3$.

*Observation* 6.7. It follows from Observation 6.2 that

(i) an odd number of factors $n_i$ with even parity and even number of factors with odd parity (or no factors with odd parity), produces additive decomposition whose summands have even parity,

(ii) otherwise, the parity of the dimensions of the summands is odd.

These observations are necessary, but not sufficient conditions to determine if a given additive decomposition corresponds to a material composition.

*Example* 6.2. Consider the additive decomposition

$$4\mathbb{C}^4 \oplus 2\mathbb{C}^6 \oplus \mathbb{C}^8 \,.$$

The total dimension is 36, which can be factorized in four ways, namely

$$36 = 6 \cdot 3 \cdot 2 = 4 \cdot 3 \cdot 3 = 9 \cdot 2 \cdot 2 = 3 \cdot 3 \cdot 2 \cdot 2 \,.$$

There is one way to decompose 36 into four factors, and three ways to decompose it into three factors. By inspecting the parity of the dimensions according to Observation 6.7 we conclude that $4 \cdot 3 \cdot 3$ is the only candidate for a tensor composition. Only this combination of factors produces even summands. However, it turns out that $4\mathbb{C}^4 \oplus 2\mathbb{C}^6 \oplus \mathbb{C}^8$ does not correspond to a tensor product of irreducible representations, since

$$\mathbb{C}^4 \otimes \mathbb{C}^3 \otimes \mathbb{C}^3 = (\mathbb{C}^2 \oplus \mathbb{C}^4 \oplus \mathbb{C}^6) \otimes \mathbb{C}^3 = 2\mathbb{C}^2 \oplus 3\mathbb{C}^4 \oplus 2\mathbb{C}^6 \oplus \mathbb{C}^8 \,.$$

That is, there is no system in Euclidean three-space that one can conceptually think of as consisting of four spin-3/2 subsystems, in addition to two spin-5/2 and a spin-7/2 subsystems. If, on the other hand, one replaces one of the four spin-3/2 subsystems with two spin-1/2 subsystems, then the corresponding material composition consists of one spin-3/2 and two spin-1 systems.

## 6.4 General check for admissibility

The terminating algorithm one can follow to determine if some additive decomposition corresponds to a tensor product of irreducible representations is the following.

If any of the steps fail, the additive composition does not correspond to a tensor product of irreducible representations.

1. Check that property 6.5 holds.
2. Check that property (6.6) holds.
3. Rearrange the additive decomposition into
   - subsums of consecutive naturals which either all have the same number of summands or the same average of the dimensions,
   - a constant subsum, i.e., a subsum whose terms are all equal. The constant subsum might consist of a single term, and it need not exist.
4. Write each non-constant subsum as a tensor product of two vector spaces. If the terms in the constant sum coincide with the common factor of the tensor product, take out the common factor out of every subsum.
5. Repeat the steps 2-4 until there is only one subsum left. If it consists of all consecutive naturals within some finite range with the same parity and unit multiplicity, write it as a tensor product.

The common divisors from the step 4 and the factors which follow from the factorization in the last step are the dimensions of the corresponding material composition. The first point of step 3 utilizes the expression (6.6) obtained for tensor product of two vector spaces. Moreover, the dimensions of the material decomposition are unique, as a consequence of uniqueness of the factors of material decomposition of two systems.

*Example* 6.3. Consider an additive decomposition

$$3\mathbb{C}^1 \oplus 6\mathbb{C}^3 \oplus 4\mathbb{C}^5 \oplus \mathbb{C}^7 \ .$$

The additive decomposition consists of all odd naturals in the range $[1,7]$. The total dimension $n = 48$ is a composite number that can be factorized in six different ways,

$$48 = 4\cdot 4\cdot 3 = 8\cdot 3\cdot 2 = 6\cdot 4\cdot 2 = 6\cdot 2\cdot 2\cdot 2 = 3\cdot 4\cdot 2\cdot 2 = 3\cdot 2\cdot 2\cdot 2\cdot 2$$

In this case we can eliminate only $6\cdot 4\cdot 2$ as a candidate, as it is the only one that produces even summands. Instead of working out the direct sum of each of the other factorizations it is quicker to follow the procedure given above. We will write only the dimensions. Conditions in step 1 and 2 hold, so we divide the sum according to step 3 as

$$\begin{aligned} 48 &= (3\oplus 3)\oplus(1\oplus 3\oplus 5)\oplus(1\oplus 3\oplus 5)\oplus(1\oplus 3\oplus 5)\oplus(3\oplus 5\oplus 7) \\ &= (3\oplus 3)\oplus(3\otimes 3)\oplus(3\cdot 3)\oplus(3\otimes 3)\oplus(5\otimes 3)\ . \end{aligned}$$

There is one constant subsum with two terms. All subsums consisting of consecutive terms have the same number of terms, three, which coincides with the terms in the constant subsum. Hence, 3 is the first common factor. After taking it out, we again rearrange the terms,

$$\begin{aligned}48 &= 3 \otimes ((1 \oplus 1) \oplus 3 \oplus 3 \oplus 3 \oplus 5) \\ &= 3 \otimes ((1 \oplus 3) \oplus (1 \oplus 3) \oplus (3 \oplus 5)) \\ &= 3 \otimes ((2 \otimes 2) \oplus (2 \otimes 2) \oplus (4 \otimes 2)) \ .\end{aligned}$$

The next common factor is 2, which leaves us with

$$\begin{aligned}48 &= 3 \otimes 2 \otimes (2 \oplus 2 \oplus 4) \\ &= 3 \otimes 2 \otimes ((2) \oplus (2 \oplus 4)) \\ &= 3 \otimes 2 \otimes ((2) \oplus (3 \otimes 2)) \ .\end{aligned}$$

Again, the common factor is 2. Finally, there is only one subsum left,

$$48 = 3 \otimes 2 \otimes 2 \otimes (1 \oplus 3) \ .$$

The terms are consecutive and of the same parity, so

$$48 = 3 \otimes 2 \otimes 2 \otimes (2 \otimes 2) \ .$$

Hence, the given additive decomposition corresponds to a tensor product of irreducible representations: The system consists of five elementry particles.

# 7 Conclusions

In this thesis, we identified a unique system theoretic additive decomposition of any materially composite quantum system in terms of independent quantum subsystems with probability ports and their interconnection through a Dirac structure.

To this end we first decomposed any given quantum system into subsystems and studied the probability flow between them. The subsystems had to be independent of each other in the sense that knowledge about the state of each separate subsystem amounts to knowledge about the state of the total system. This immediately means that the subsystems cannot be given by the individual tensor factors that describe the Hilbert space of a materially composed quantum system. This is because the tensor product of Hilbert spaces contains elements, so-called entangled vectors, that cannot be described in terms of one element from each Hilbert space in the tensor factor. The identification of the Hilbert spaces underlying suitable independent subsystems required a careful understanding of the role of the physical space in which the quantum system is situated, which furnishes each Hilbert space with additional structure in the form of a representation of the isometry group of the underlying space. It is this additional structure that allowed us to decompose any tensor product of Hilbert spaces into a unique direct sum, whose summands constitute the Hilbert spaces underlying the otherwise elusive independent subsystems. It was then straightforward to rewrite Schrödinger's equation for a composed quantum system as a system of coupled equations, one for each subsystem. In turn, writing these equations in input-output form allowed the identification of a probability flow between the independent subsystems as a real-valued inner product between input and output. Despite superficial appearances, this input-output form did not immediately lend itself to a description of the total system in terms of the identified independent subsystems and their interconnection via a Dirac structure through ports. This is because the port, by which each subsystem connects to the Dirac structure, must be independent of the number and nature of the ports of other subsystems that connect to the same Dirac structure. The solution consists in shifting the input matrices of all subsystems into one single Dirac structure that has as many ports as there are independent subsystems. Each of these ports is then defined exclusively in terms of the Hilbert space of the respective independent subsystem. Interconnection of this Dirac structure to each subsystem then constitutes the sought-for formulation in terms of probability ports and a Dirac structure. The value of this decomposition consists in its modularity: Removing one subsystem from the originally closed system results in a system with a free port. Connecting this free port to one other subsystem or, via a further intermediate Dirac structure, to several other subsystems, an entirely new quantum system may be obtained. If one insists, as one physically may well do, that the resulting quantum system, can be thought of as consisting of elementary particles only, there are combinatorial constraints on the subsystems that can be added in this way. We presented a terminating algorithm to determine the admissibility of such modular extensions.

The insights gained and results presented in this thesis immediately prompt several interesting questions for further research. We mention three of those, in descending order of difficult.

First, how could one incorporate the second dynamical mechanism present in quantum mechanics, namely the projective dynamics at any time of measurement, into the formalism? The dual nature of a measurement apparatus, which connects an observer's knowledge about the state of a quantum system with the same observer's classical knowledge of the measurement result, makes this a conceptually highly interesting and relevant question. The development of a hybrid formulation that negotiates the switch between the unitary dynamics discussed in this thesis on the one hand and the projective dynamics of a measurement apparatus on the other hand appears to be a first obvious step, but is likely to be informed in detail again by the postulates of quantum mechanics rather than any formal analogy to the hybrid port-Hamiltonian theory. An exciting prospect would be the possibility to shed some new light on the formulation of the measurement problem of quantum mechanics.

Second, how can the the formalism be extended such as to deal with submaximal knowledge? This is required if one wishes to incorporate observers who voluntarily or involuntary fail to read off the result shown by some measurement apparatuses. The technical treatment of submaximal knowledge will likely further refine the formalism and may well play a role in the solution to the incorporation of measurements mentioned before.

Third, how do our results generalise to systems with translational degrees of freedom? This will necessarily require to employ the full apparatus of functional analysis in order to deal with an infinite-dimensional Hilbert space and unbounded operators. Another interesting technical extension would be to translate the results of this thesis to the universal covering group $SL(2,\mathbb{C})$ that governs relativistic particles without translational degrees of freedom and to study which insights, if any, will be afforded in that area by use of the additive decomposition formalism.

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