

BSc Thesis Applied Mathematics - Applied Physics

Kinematic decomposition of quantum systems

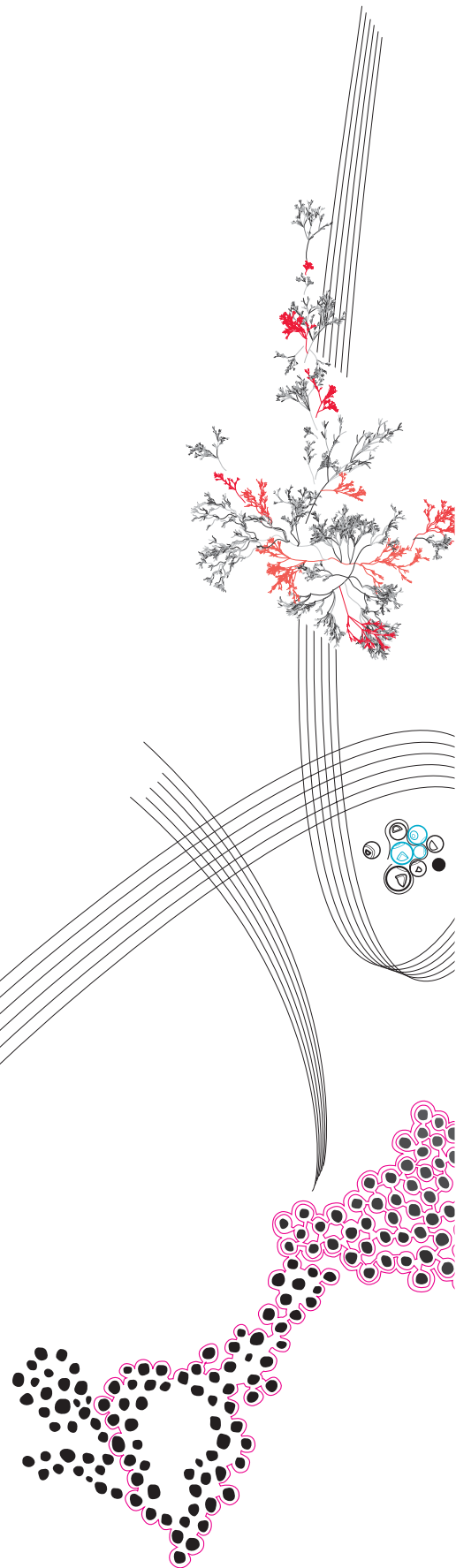
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Preface

Firstly, I want to thank Kia Romero Hojjati, my Mexican camarada, with whom I worked almost daily. You elevated this research to new heights and I learned a lot from your mathematical point of view and your — sometimes so annoying — rigour.

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Abstract

Standard descriptions of both classical physics, as described by Hamiltonian dynamics, and quantum physics, as described by unitary dynamics, describe closed systems. Their formalism excludes the possibility of describing systems which exchange energy with their surroundings. In classical physics, this issue is remedied by port-Hamiltonian theory, which allows to describe open systems and their interaction with each other. In quantum mechanics no such comprehensive theory of open systems exists. Quantum systems are much harder to compose and decompose due to the tensor product constructions, by which the composition of quantum systems are defined. In this thesis, we successfully address the kinematic part of this problem by exploitation of the fact that any tensor product composition of finite-dimensional quantum systems can be rewritten as a direct sum decomposition. A unique such direct sum decomposition is obtained by considering, without loss of generality, only fundamental quantum systems whose Hilbert spaces are reducible or irreducible representations of $SU(2)$. The description of the dynamics of a quantum system that is decomposed in quantum port-Hamiltonian fashion can now be erected on this result and is briefly touched upon.

Keywords: open quantum systems, quantum symmetries, port-Hamiltonian theory

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1 Introduction

Standard descriptions of classical physics, as described by Hamiltonian dynamics, and quantum physics, as described by unitary dynamics, describe *closed* systems. Closed means that not only is there no interaction with another system. The impossibility to exchange energy is, in fact, encoded at the heart of the respective formalisms. Indeed, the double role of the classical Hamiltonian function as both the generator of time evolution on the one hand, and as the energy observable on the other hand means that¹

$$\dot{H} = \{H, H\},$$

which then, by the antisymmetry of the canonical Poisson bracket $\{\cdot, \cdot\}$, inevitably implies

$$\dot{H} = 0$$

for any such system. Similarly, in the Heisenberg picture of quantum mechanics, where operators representing as quantum observables carry the time evolution of the system, the time evolution is given by

$$\dot{\hat{H}} = \frac{i}{\hbar}[\hat{H}, \hat{H}] = 0$$

in terms of the antisymmetric commutator bracket $[\cdot, \cdot]$ and thus again reveals an inherently *closed system*. This means that neither the Hamiltonian formalism for classical nor the standard formulation of quantum systems is able to describe subsystems of a closed system, unless each of these themselves are energetically closed and thus do not exchange energy with each other. In other words, the Hamiltonian formulation requires to model a closed system ‘as a whole’, rather than as a composition of mutually exchanging subsystems.

For the modelling of simple physical systems with few degrees of freedom, such a holistic modelling ultimately amounts to reverse engineering: both the choice of state space and the choice of Hamiltonian are made such as to yield the observed behaviour of the system. For the case of a pointlike mass m in non-relativistic classical physics, for instance, one models the Hamiltonian as

$$H(q, p) := \frac{p^2}{2m},$$

where $q \in \mathbb{R}$ and $p \in \mathbb{R}$ are the position and the momentum of the particle respectively². The Hamiltonian evolution of the position of the particle then yields the uniform straight motion laid down in Newton’s first law, and, much more importantly, the observed behaviour of such a system under idealized laboratory conditions. Thus one obtains the Hamiltonian theory of a single free mass as a *closed system*. Similarly, one may model a Hooke spring of mass μ , spring constant k , and very short rest length ℓ . Usually one does not model a spring by itself, describing its actual mechanics, but by prescription of an effective potential whose gradient yields the force that the spring exerts on a mass. If we were to model a spring on its own, however, for once modelling it as an object with mass, we may consider its mass μ to be much smaller than the mass m of any pointlike particle, we intent to connect it to. This way, the spring-mass will not have a significant effect, as is usually assumed. By pretending that the mass is distributed in equal parts to the endpoints one may then model the Hamiltonian of such a spring as

$$H(q_1, q_2, p_1, p_2) := \frac{p_1^2}{\mu} + \frac{p_2^2}{\mu} + \frac{k}{2}(q_2 - q_1 - \ell)^2$$

¹Properly written, the temporal rate of change law for an observable F along a phase space trajectory X reads $\frac{d}{dt}(F \circ X) = \{F, H\} \circ X$. This is often notationally condensed to $\dot{F} = \{F, H\}$ as used here.

²We choose the smallest possible classical mechanical phase space here in order to illustrate the conceptual points we wish to make. All conclusions generalize to general Hamiltonian systems.

where $q_1, q_2 \in \mathbb{R}$ are the left and right endpoints of the spring respectively and $p_1, p_2 \in \mathbb{R}$ are its momenta. This Hamiltonian is the simplest description of the behaviour of an isolated physical spring. Indeed, the naive modelling folklore, that an isolated spring somehow corresponds to just a potential $V(q) = \frac{1}{2}k(q - \ell)^2$, produces an inconsistent Hamiltonian system, since $H(q, p) = V(q)$ implies $\dot{q} = 0$ and $\dot{p} = -k(q - \ell)$, which would describe a spring whose elongation can not change while its momentum grows arbitrarily for $q \neq \ell$.

Hence also just folklore within Hamiltonian theory is the idea that two masses, that are attached to both ends of a spring, would somehow transfer their ‘kinetic’ energies to each other via the ‘potential’ energy of the spring. Not only is the formalism of Hamiltonian theory no more able to distinguish between the kinetic energy T and the potential energy V in $H = T + V$ than the algebra of natural numbers is able to uniquely decompose 5 into $2+3$ rather than $1+4$. But the Hamiltonian formalism is also not able to magically convert its inevitably *closed system* descriptions of a free mass and an isolated spring into open subsystem descriptions, which would be required to underpin the folklore that maintains that the masses and the spring exchange energy. Indeed, this idea is in direct conflict with the basic structure of both the classical and quantum Hamiltonian formalisms.

The modelling of Hamiltonians for intuitively composed systems thus can not be a well-defined formal procedure but ultimately proceeds by rules of thumb and by experience, one developed some intuition for the observed and desired result. In other words, the standard descriptions of classical physics and quantum physics do not provide a rigorous theory for the composition of systems. This severe theoretical problem is not much of a practical problem as long as one considers only small and simple physical systems. But for large complex systems, this lack of a formal way to describe open subsystems and their interconnection becomes a serious practical liability of the standard formulations.

For classical physics there exists port-Hamiltonian theory which can rigorously describe open subsystems and their interconnection. This is a largely worked out theory and is used in high-level engineering and numerical modelling of physical systems. Its full power unfolds in the consideration of large complicated systems such as a nation or continent-wide power grid or modern robotics. Since classical port-Hamiltonian theory — a description of subsystems which allows energy exchange with other subsystems that ensures overall energy conservation and a formal theory of interaction of such subsystems — requires conceptually and technically an entirely different implementation in its classical setting than will be required in the quantum setting we consider in this thesis, it is not useful to provide a review of the classical port-Hamiltonian theory and we will not do so.

It is the aim of this thesis to implement the essential idea of port-Hamiltonian theory in quantum mechanics. As classical physics and quantum mechanics vastly differ, we can only consider the basic ideas that underlie port-Hamiltonian theory, rather than its existing conceptual and technical implementation. In our review of quantum mechanics in chapter 2, following from the fourth axiom of quantum mechanics, we will encounter the difficulties that arise from composing quantum systems with a tensor product. As the composition and decomposition of systems is of central importance for a construction of a port-Hamiltonian theory of quantum mechanics, the inability to decompose combined quantum systems is the central problem of this thesis.

After chapter 2, we will provide a direct sum decomposition of the Hilbert spaces of composed quantum systems, by considering only fundamental quantum systems. This decomposition identifies the state spaces for the subsystems in which the composed system can be decomposed in port-Hamiltonian fashion. Since it is valid (and indeed a prerequisite) for all possible dynamical decompositions built on it, we will refer to it more precisely as a kinematic decomposition. We however touch upon dynamic decompositions in chapter 4.

2 The foundation of quantum mechanics

In order to construct a formalism for quantum mechanics which is able to describe open subsystems such that their composition, to one closed system, is compatible with the standard axioms of quantum mechanics for closed systems, we now first review the latter. As stated in the first axiom, the underlying mathematical structure of quantum mechanics is a Hilbert space and the rest of quantum theory will be modelled upon such space. This research will only focus on finite-dimensional Hilbert spaces, restricting our attention in this thesis to finite-dimensional quantum systems. In this chapter, we will look at the mathematical framework of quantum mechanics, especially: the state space of quantum mechanics, the dynamics of a quantum system, measurement in quantum mechanics, and the composition of quantum systems.

2.1 The state space of quantum mechanics

In this section, we start by defining the mathematical framework necessary to model a quantum system. Additionally, we will define the general state space of quantum mechanics and define quantum states in this section.

Axiom 1. Associated to any isolated quantum system is a separable Hilbert space³ $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ with a complex Hermitian inner product $\langle \cdot | \cdot \rangle$. The choice of Hilbert space is a question of physical modelling.

Now that we have defined the underlying mathematical space of quantum mechanics, we are interested in describing a quantum system, which is done by defining a quantum state⁴.

Definition 1. The state of a quantum system, at any particular time, is given by a linear map $\rho : \mathcal{H} \rightarrow \mathcal{H}$ which is:

- (i) Hermitian: $\forall \psi \in \mathcal{H} : \langle \rho(\psi) | \psi \rangle = \langle \psi | \rho(\psi) \rangle$
- (ii) non-negative: $\forall \psi \in \mathcal{H} : \langle \psi | \rho(\psi) \rangle \geq 0$
- (iii) normalized: $tr(\rho) = 1$.

In quantum mechanics there exist two different kinds of states: pure states and mixed states. Mathematically, the two types of states can be classified by $tr(\rho^2) = 1$ for pure states and $tr(\rho^2) < 1$ for mixed states. As we will see in axiom 3, one can not predict the outcome of a measurement. Yet, measurement will spontaneously alter the quantum state depending on the measurement outcome. It is possible, however, to perform a measurement, thereby collapsing the state to a new state, and to not obtain the measurement result. This is called ‘classical ignorance’ as the observer does not obtain the information from the measurement apparatus and generates a mixed state. Pure states are states with no classical ignorance and are convenient to work with as they can be uniquely expressed by elements of the Hilbert space. These elements, which are called ‘the state vectors’ ψ or $|\psi\rangle$, are often much easier to work with.

Lemma 1. A pure state can be uniquely determined by a state vector $\psi \in \mathcal{H}$ such that

$$\rho_{pure} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \quad (2.1)$$

³As mentioned previously we will restrict our attention to finite-dimensional Hilbert spaces. It is also important to note that the standard convention in quantum mechanics is to take the inner product to be antilinear in the first slot.

⁴The following definition of a state is often also called a ‘density operator’.

Proof. Since ρ is a Hermitian map there exists an orthonormal basis such that we can express ρ by its spectral decomposition $\rho = \sum_{i=1} \lambda_i |i\rangle\langle i|$, where λ_i are its eigenvalues and $|i\rangle$ the respective eigenvectors. Since ρ is a pure state, $\text{tr}(\rho) = \text{tr}(\rho^2) = 1$,

$$\begin{aligned} \text{tr}(\rho) &= \sum_n \langle n|\rho|n\rangle = \sum_n \sum_i \lambda_i \langle n|i\rangle\langle i|n\rangle = \sum_n \sum_i \lambda_i \delta_{n,i} = \sum_i \lambda_i = 1, \\ \text{tr}(\rho^2) &= \sum_n \sum_i \lambda_i^2 \langle n|i\rangle\langle i|n\rangle = \sum_i \lambda_i^2 = 1. \end{aligned}$$

Therefore, the difference of the traces is given by $\sum_i \lambda_i(1 - \lambda_i)$. Since ρ is a positive operator its eigenvalues must be positive and therefore it is only possible to have one $\lambda_k = 1$ while all others must be zero. Lastly, since arbitrary Hilbert space elements are not normalized, we introduce a normalization factor in the denominator. \square

From this proof, it is clear that even though we prefer to talk about states ρ , in the pure case, we may equivalently work with the state vectors ψ as they uniquely generate the state ρ_ψ . Note that the converse is not true, there does not exist a state vector ψ for every state ρ . It is the mixed states, which arise from classical ignorance, that can only be described by some ρ , but not in terms of a state vector ψ . Although the state of a quantum system is commonly defined in many undergraduate textbooks as the elements of the Hilbert space, this only captures pure states as they can be generated from the state vectors as given Eq.2.1. To fully capture all possible states in quantum mechanics we must adhere to the definition of a state as given in definition 1.

2.2 The dynamics of quantum systems

Now that we have defined the general state space of quantum mechanics, defining states at any particular time as linear maps on the underlying Hilbert space, we are interested in their time evolution. In this section, we will define what quantum observables are and give the axiom that describes the time evolution of quantum states in closed quantum systems.

Definition 2. A quantum observable is a physically measurable quantity \mathcal{A} and is described by a Hermitian operator A acting on the Hilbert space \mathcal{H} of the system.

Since the operators that describe quantum observables are Hermitian they have real eigenvalues, and as we will see in the next section, these eigenvalues are the measurement outcomes when measuring a physical quantity. Similar to the energy observable in classical physics, quantum mechanics has an energy observable called ‘the Hamiltonian’, a Hermitian operator $\hat{H} : \mathcal{H} \rightarrow \mathcal{H}$. Again similar to classical physics, this Hamiltonian plays an important role in the time evolution of quantum mechanics.

Axiom 2. The time evolution of a quantum state in a closed quantum system is described by the Schrödinger equation

$$\dot{\rho}(t) = \frac{-i}{\hbar} [\hat{H}, \rho(t)], \quad (2.2)$$

where \hbar is a physical constant called Planck’s constant, \hat{H} the Hamiltonian, and $[\cdot, \cdot]$ the commutator bracket which is defined by the composition of linear maps on the Hilbert space $[A, B] = A \circ B - B \circ A$.

Alternatively, one can give a discrete time evolution of the state from time t_1 to time t_2 by describing a unitary map $U(t_1, t_2)$ such that the system's state $\rho(t_2)$ at time t_2 is obtained from the state $\rho(t_1)$ at time t_1 by virtue of

$$\rho(t_2) = U(t_1, t_2)\rho(t_1)U(t_1, t_2)^\dagger, \quad (2.3)$$

where \dagger is used to denote the conjugate transpose. The relation between the unitary map $U(t_1, t_2)$ and the Hamiltonian operator is then given by

$$U(t_1, t_2) = e^{\frac{-i\hat{H}(t_2-t_1)}{\hbar}}. \quad (2.4)$$

As previously mentioned, often only pure quantum states are considered. Since, in that case, we can uniquely determine the state from the state vectors, a specific case of the Schrödinger equation can be used

$$i\hbar\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle. \quad (2.5)$$

Again, as this does not capture all states in quantum mechanics, namely it ignores the presence of mixed states, it is merely a special case of axiom 2.

2.3 Measurement in quantum mechanics

The previously given description of time evolution of a state only concerns the time evolution of a state in a closed quantum system. In this section, we will see how measurement in quantum mechanics will give an alternative time evolution that instantaneously changes the state. Additionally, we will look at quantum measurement and the importance of probability in quantum measurement.

Axiom 3. All measurements in quantum mechanics, often called projective measurements, are observables described by a Hermitian operator $M : \mathcal{H} \rightarrow \mathcal{H}$ which has a spectral decomposition

$$M = \sum_{m \in \text{Spec}(M)} m P_{\text{eig}_m(M)}, \quad (2.6)$$

where $P_{\text{eig}_m(M)}$ is an orthogonal Hermitian projector to the eigenspace of M for the respective eigenvalue m . Only the elements $m \in \text{Spec}(M) \subset \mathbb{R}$ are possible measurement outcomes. One can not predict which $m \in \text{Spec}(M)$ will be measured, only the probability for a measurement to yield the definitive value m

$$p(m|\rho^-) = \text{tr}(P_m \rho^-), \quad (2.7)$$

where ρ^- is the state right before the measurement takes place. Only by actually measuring the state, ρ^- will collapse into the new state

$$\rho^+ = \frac{P_{m_{\text{obs}}} \rho^- P_{m_{\text{obs}}}}{\text{tr}(P_{m_{\text{obs}}} \rho^-)}, \quad (2.8)$$

where m_{obs} is the observed measurement result[1].

Of course, by definition, the total probability of measuring all possible measurement outcomes must be equal to one and indeed this simply follows from the definition given in the axiom:

$$\sum_m p(m|\rho^-) = \sum_m \text{tr}(P_m \rho^-) = \text{tr}\left(\sum_m P_m \rho^-\right) = \text{tr}(\rho^-) = 1,$$

where we used that the sum of all eigenprojectors is equal to the identity, that the trace is linear, and that states are normalized.

A subtle consequence of Axiom 3, is the generation of mixed states by not reading off a measurement. Indeed, if one performs a measurement on a quantum system such that its state collapses, but the observer does not look at the measurement apparatus, the observer creates classical ignorance and the state collapses into a mixed state. Since the observer did not look at the measurement outcome, one can only conclude the collapsed state will be a mixture of all possible measurement state outcomes with their respective probability. The mixed state can thus be described by

$$\rho^+ = \sum_m p(m|\rho^-) \frac{P_m \rho^- P_m}{\text{tr}(P_m \rho^-)} = \sum_m P_m \rho^- P_m. \quad (2.9)$$

The previously introduced Hamiltonian also functions as the energy observable in quantum mechanics. It is an observable just like the M observable given in axiom 3 and its eigenvalues are the possible energy values of the system. Although one could recognize some similarities between the classical and quantum Hamiltonian, it being the generator of time evolution in the Schrödinger equation and the energy observable, this comparison must be taken with a grain of salt as they are very different mathematical objects with very different properties.

This section has provided us with a second time evolution. If a state in a closed quantum system evolves with time it does so according to Eq.2.2. If the system is measured, however, the state collapses instantaneously, as opposed to the unitary time evolution for a closed quantum system, resulting in a new state as given axiom 3.

2.4 The composition of quantum systems

For a proper theory of interaction in quantum mechanics, analogous to the classical implementation of port-Hamiltonian theory, it is of central importance to understand how systems are composed. In quantum mechanics, the composition of quantum systems is realized by taking the tensor product of constituent subsystems, resulting in the composed system having a dimension which is the product of the dimensions of its constituents. This composition of systems results in a state space that contains states that cannot be understood anymore in terms of states of the constituent subsystems. This loss of information, following from the axioms of quantum mechanics, is a central problem when trying to construct a theory that requires the combining and decoupling of quantum systems.

Axiom 4. Given two quantum systems with underlying Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , the composite quantum system has $\mathcal{H}_A \otimes \mathcal{H}_B$ as its underlying Hilbert space.

As the dimension of two Hilbert spaces composed by a tensor product is the dimension of the individual Hilbert spaces multiplied by each other, composing a Hilbert space of dimension m with a Hilbert space of dimension n will result in a Hilbert space of dimension nm . Since the dimension of the combined Hilbert space (in almost all cases) is higher than the sum of the dimensions of the constituent Hilbert spaces, the combined Hilbert space can contain states that can not be expressed in the separate constituent systems. Such states are called ‘entangled states’ and their existence makes a simple decomposition of $\mathcal{H}_1 \otimes \mathcal{H}_2$ into \mathcal{H}_1 and \mathcal{H}_2 nonsensical.

By the structure provided in axiom 4, composing two states ρ_A and ρ_B from two different systems is defined by taking their tensor product such that $\rho_{AB} = \rho_A \otimes \rho_B$. This then leads to the following definition of entangled states.

Definition 3. A composed state is entangled if it can not be described as a single tensor product of quantum states.

Since the tensor product of two Hilbert spaces (almost always) has a higher dimension than the sum of the dimensions of its constituent Hilbert spaces, these entangled states can exist in the composed Hilbert space but do not exist in the individual constituent Hilbert spaces. In the case of pure states, for example, given state vectors $\psi_1, \psi_2 \in \mathcal{H}_1$ and $\phi_1, \phi_2 \in \mathcal{H}_2$, we can, at this point, make no sensible remark how the entangled state vector $\psi_1 \otimes \phi_2 + \psi_2 \otimes \phi_1 \in \mathcal{H}_1 \otimes \mathcal{H}_2$ would correspond to state vectors in the original Hilbert spaces and therefore decomposing the statespace of $\mathcal{H}_1 \otimes \mathcal{H}_2$ into \mathcal{H}_1 and \mathcal{H}_2 is impossible. It is important to note that classically, the composition of two systems is merely the thought of thinking of two systems as one, nothing changes within the systems except our conceptual notion of what we define as a system. According to this axiom, whether we consider two separate quantum systems or consider them as a single (larger) system matters, as these considerations differ. This is problematic for our conceptual notion of what we define as a quantum system and for a port-Hamiltonian theory of quantum mechanics which would require the repeated composition, but also decomposition of (open) systems. This lack of a simple decomposition of quantum systems, therefore, is the central problem of this thesis, which directly stems from the fourth axiom of quantum mechanics.

3 Kinematic decomposition of quantum systems

As seen in chapter 2, the composition of two quantum systems occurs by composing their associated Hilbert spaces with a tensor product. The tensor product structure allows for the existence of entangled states in quantum mechanics, which largely complicates a simple decomposition of the composed Hilbert spaces. As a port-Hamiltonian theory of quantum mechanics would require the coupling and decoupling of multiple (open) subsystems, this issue is the central problem of this thesis. There do exist certain methods for subdividing quantum systems, e.g. the partial trace and purification, yet non of these methods, by construction, preserve all the states that describe the system. In this chapter, we will clearly present the problem that arises from the tensor product composition as stated in the axioms of quantum mechanics. A solution to this problem is to express the composed Hilbert spaces, by their isomorphisms, as a direct sum of Hilbert spaces. Yet, by using the Hilbert space isomorphisms there exist many possible configurations of this decomposition. In order to resolve this ambiguity and to rightfully decompose the Hilbert spaces, we will consider fundamental quantum systems, which model quantum systems by using all information possibly available. This will lead us to the fundamental symmetry of non-relativistic quantum mechanics and will help us find a unique such direct sum decomposition. As we still only consider finite-dimensional Hilbert spaces, we will focus our attention to spin systems which describe the spin of a particle. The main result of this chapter is a complete decomposition of composed finite-dimensional fundamental quantum systems into a direct sum of finite-dimensional fundamental quantum systems. This decomposition rightfully constitutes a ‘kinematic decomposition’ and describes how to decompose the state spaces as well as the state vectors of finite-dimensional fundamental quantum systems.

3.1 The inability to decompose quantum systems

In chapter two, we discussed the composition of quantum systems and introduced the definition of ‘entangled states’. In this section, we will restate the central problem of this thesis on how to compose and decompose quantum systems and we will provide our main idea on how to solve this problem. The following sections will build on this idea and by the end of this chapter, this idea will lead to the construction of a complete kinematic decomposition of finite-dimensional fundamental quantum systems. As stated previously, we will focus on finite-dimensional quantum systems, which as we will see in this section, are equivalent to quantum spin systems.

As stated in the fourth axiom of quantum mechanics, the composition of two quantum systems occurs by composing their associated Hilbert spaces with a tensor product. Since the tensor product effectively multiplies the dimension of the composed Hilbert spaces, the sum of the dimensions of the constituent Hilbert spaces is (almost always) smaller than the dimension of their composed Hilbert space. As introduced in chapter 2, this allows for the existence of entangled states, states that can exist in the composed Hilbert space, due to its larger dimension, but can not be expressed in the individual Hilbert spaces. This problem does not arise when composing two Hilbert spaces with a direct sum as a direct sum composed Hilbert space has the same dimension as the sum of the dimensions of its constituent Hilbert spaces. Additionally, the composition by a direct sum, by definition, maintains separate independent Hilbert spaces.

As stated before, we will only consider finite-dimensional quantum systems, i.e. quantum systems whose associated Hilbert spaces are finite-dimensional. The Hilbert space of any non-relativistic quantum system can be modelled by $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^n$, where $L^2(\mathbb{R}^3)$

is associated to the movement of the particle and \mathbb{C}^n describes the spin of a particle. In order to only consider finite-dimension Hilbert spaces, therefore, we must consider quantum systems with no translational degrees of freedom, i.e. we ignore, without loss of generality, the first part of the Hilbert space. From this consideration, it follows that when we are considering finite-dimensional quantum systems we will always be modelling spin, with Hilbert space $\mathcal{H} = \mathbb{C}^n$, and often refer to such finite-dimensional quantum systems as ‘spin systems’.

Spin is a property carried by all fundamental particles and the spin of a particle is given by a positive number (including zero) which is either an integer or half-integer. When measuring the spin of a particle with spin $s \in \frac{\mathbb{N}_0}{2}$, there are $2s + 1$ possible measurement outcomes m ranging from s to $-s$ in steps of one. Therefore, in order to model the spin of such a particle requires a Hilbert space $\mathcal{H} = \mathbb{C}^{2s+1}$, which contains $2s+1$ orthonormal basis vectors, one for each possible measurement outcome, and allows for complex linear combinations. We then choose a specific basis such that the basis vectors are eigenvectors of the S_z operator, which in this basis will be a diagonal matrix with eigenvalues m ranging from s to $-s$ in steps of one. Since these eigenvalues m , often called ‘the spin level’ or ‘magnetic quantum number’, of the S_z operator are also the possible measurement outcomes, this choice of basis makes S_z the spin level measurement observable. So these eigenvalues m can be obtained by applying the S_z operator to a Hilbert space basis element commonly denoted as $|s\ m\rangle \in \mathcal{H}$,

$$S_z |s\ m\rangle = m |s\ m\rangle. \quad (3.1)$$

In this notation $|s\ m\rangle = |\frac{3}{2} - \frac{1}{2}\rangle$ would describe a spin-3/2 system, which can be modelled with $\mathcal{H} = \mathbb{C}^4$ with a basis of four eigenvectors of S_z , and the basis vector corresponding to the spin level $-1/2$.

As a consequence of modelling finite-dimensional Hilbert spaces by $\mathcal{H} = \mathbb{C}^n$, we could decompose the Hilbert spaces of composed spin systems by using their isomorphisms

$$\mathbb{C}^n \otimes \mathbb{C}^m \cong \underbrace{\mathbb{C} \oplus \mathbb{C} \oplus \dots \oplus \mathbb{C} \oplus \mathbb{C}}_{n \times m \text{ times}}.$$

By expressing the Hilbert spaces up to isomorphisms, we seem to implicate that we can express the Hilbert spaces composed by a tensor product in many different configurations of direct sums of Hilbert spaces

$$\mathbb{C}^3 \otimes \mathbb{C}^2 \cong \mathbb{C}^6 \cong \mathbb{C}^5 \oplus \mathbb{C}^1 \cong \mathbb{C}^3 \oplus \mathbb{C} \oplus \mathbb{C}^2.$$

This decomposition is purely based on mathematical arguments and to investigate which configurations of direct sum decompositions are possible we will consider fundamental quantum systems. When fundamentally modelling a quantum system we incorporate all known information of that system without simplifying or neglecting any information. This will allow us to consider all possible knowledge of quantum systems and to give physical arguments for why certain configurations of direct sum decompositions are not possible.

3.2 Fundamental quantum systems

When modelling any physical system one has the option to model a system fundamentally or to give a merely effective model of the system. A fundamental model incorporates all details of the system at the level of current knowledge. A merely effective model, in contrast, takes the freedom to summarize the effect, of an often much more complex physical situation, in order to provide a simplified description that is assumed to suffice for a particular question of interest. As effective models typically break the symmetry that a fundamental

description possesses and we are interested in describing fundamental quantum systems, this section will focus on the underlying symmetries of quantum mechanics and how they can be incorporated into quantum theory to model fundamental quantum systems.

In physics, the conservation of a physical quantity is the result of an underlying symmetry of the physical system. In quantum mechanics, when we do not consider the translational degrees of freedom of a particle as described in the previous section, spin is a conserved quantity. The fundamental symmetry of non-relativistic quantum mechanics, therefore, is $SU(2)$ as its representations are able to describe particle spin [2]. In order to use elements of the symmetry group $SU(2)$ as quantum operators acting on some Hilbert space requires the use of representation theory. In this thesis, we will mainly focus on the application of representation theory of $SU(2)$. $SU(2)$ is known as a Lie group, but as we want to use it for practical purposes, it will not be important to have any additional knowledge of Lie groups. Alternatively, we will define the group $SU(2)$ and work with the given definition

$$SU(2) \equiv \left\{ \begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix} \mid \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1 \right\}. \quad (3.2)$$

With this definition, $SU(2)$ is the special unitary group of unitary 2×2 matrices with determinant 1 where the group operation is matrix multiplication. Associated to the group $SU(2)$ is a Lie algebra, a vector space with an additional bilinear map, but we will, again, only work with the given definition. This associated Lie algebra, called $su(2)$, is useful as it is often much easier to work with than its group $SU(2)$

$$su(2) \equiv \left\{ \begin{pmatrix} ia & b+ic \\ -b+ic & -ia \end{pmatrix} \mid a, b, c \in \mathbb{R} \right\}. \quad (3.3)$$

Hence, $su(2)$ describes the vector space of 2×2 anti-Hermitian matrices with trace zero where the Lie bracket is defined as the commutator bracket of these matrices. A possible basis for $su(2)$ is

$$E_1 = \frac{1}{2} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \quad E_2 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad E_3 = \frac{1}{2} \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

The Lie group elements of $SU(2)$ and the associated Lie algebra elements are related such that the group elements can be obtained from the algebra elements by

$$\hat{R}_j = e^{E_j \theta}.$$

where $\hat{R}_j \in SU(2)$ and $E_j \in su(2)$. Conversely, one obtains the algebra elements of $su(2)$ from $SU(2)$ by

$$E_j = \left. \frac{\partial \hat{R}_j}{\partial \theta} \right|_{\theta=0} \quad j = 1, 2, 3.$$

As shown in [2], $SU(2)$ is the fundamental symmetry group for non-relativistic finite-dimensional quantum systems, but in order to use these group and algebra elements on the Hilbert spaces of quantum theory we must turn to representation theory.

Definition 4. A finite-dimensional linear representation of the Lie algebra $su(2)$ is a linear map

$$\rho : su(2) \longrightarrow \text{End}(V)$$

with the property

$$\rho(\llbracket l_1, l_2 \rrbracket) = [\rho(l_1), \rho(l_2)].$$

Here $\llbracket \cdot, \cdot \rrbracket$ defines the commutator bracket of $su(2)$ matrices, V is some finite-dimensional vector space, called the representation space and $[\cdot, \cdot]$ is the commutator bracket, which is defined by the composition of maps $\phi, \psi \in \text{End}(V)$ such that $[\phi, \psi] := \phi \circ \psi - \psi \circ \phi$. It is often easier to work with the associated Lie algebra $su(2)$ and its representations, yet we do also need the definition of a linear representation of the group $SU(2)$.

Definition 5. A finite-dimensional linear representation of the Lie group $SU(2)$ is a linear map:

$$\Gamma : SU(2) \longrightarrow GL(V)$$

such that

$$\Gamma(g_1) \circ \Gamma(g_2) = \Gamma(g_1 g_2),$$

where

$$GL(V) := \{\varphi \in \text{End}(V) \mid \det(\varphi) \neq 0\}.$$

An important subspace of representations are the ‘irreducible representations’.

Definition 6. If $\Gamma : SU(2) \rightarrow GL(V)$ is a representation of $SU(2)$, then if $\exists W \subseteq V$ such that $\forall g \in SU(2), \Gamma(g)w \in W \forall w \in W$, Γ is an irreducible representation of $SU(2)$ if and only if $W = 0$ or $W = V$.

In other words, the representation can not be made into smaller representations and is therefore an irreducible representation — often abbreviated to ‘irrep’.

Now that we have defined linear representations of both $SU(2)$ and $su(2)$ we can find the spin matrices which are used to describe spin

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (3.4)$$

where these 2×2 Hermitian spin matrices follow from the $su(2)$ representation $\rho(E_i)$ such that

$$S_i = i\hbar\rho(E_i), \quad (3.5)$$

with the commutation relations

$$[S_x, S_y] = i\hbar S_z, \quad [S_z, S_x] = i\hbar S_y, \quad [S_y, S_z] = i\hbar S_x. \quad (3.6)$$

The third spin matrix, S_z , is the spin operator used in the last section, where its eigenvalues give the different spin levels. It might be of interest to raise the spin level in a spin system, effectively changing from one basis element to another. This can be done with the ladder operators

$$\begin{aligned} S_+ &= S_x + iS_y \\ S_- &= S_x - iS_y, \end{aligned} \quad (3.7)$$

such that

$$S_{\pm}|s m\rangle = \sqrt{s(s+1) - m(m \pm 1)} |s m \pm 1\rangle. \quad (3.8)$$

These operators also ensure that when the highest spin level is raised or the lowest spin level is lowered the statevector $|s m\rangle$ will be annihilated. As S_x and S_y are defined by representations of $su(2)$ as given in Eq.3.5, similarly S_+ and S_- can be defined by representations of $su(2)$.

Definition 7. Suppose (Γ_1, V_1) and (Γ_2, V_2) are two representations of $SU(2)$. The direct sum of these two representations: $\Gamma_1 \oplus \Gamma_2 : SU(2) \rightarrow GL(V_1 \oplus V_2)$ is given by

$$(\Gamma_1 \oplus \Gamma_2)(A) = \Gamma_1(A) \oplus \Gamma_2(A).$$

The tensor product of Γ_1 and Γ_2 is the representation $\Gamma_1 \otimes \Gamma_2 : SU(2) \rightarrow GL(V_1 \otimes V_2)$ given by

$$(\Gamma_1 \otimes \Gamma_2)(A) = \Gamma_1(A) \otimes \Gamma_2(A)$$

Similarly the direct sum and tensor product of Lie algebra representations can be defined as

$$\begin{aligned} (\gamma_1 \oplus \gamma_2)(X) &= \gamma_1(X) \oplus \gamma_2(X) \\ (\gamma_1 \otimes \gamma_2)(X) &= \gamma_1(X) \otimes I_2 + I_1 \otimes \gamma_2(X), \end{aligned}$$

where I_1 and I_2 are the identities in the respective representation spaces [2].

This now allows us to define the ladder operators and S_z for composed finite-dimensional quantum systems

$$\begin{aligned} S_+^{(tot)} &= S_+^{(m)} \otimes I_n + I_m \otimes S_+^{(n)} \\ S_-^{(tot)} &= S_-^{(m)} \otimes I_n + I_m \otimes S_-^{(n)} \\ S_z^{(tot)} &= S_z^{(m)} \otimes I_n + I_m \otimes S_z^{(n)}, \end{aligned} \quad (3.9)$$

where $S^{(tot)}$ denotes operators on the composed Hilbert space $\mathbb{C}^m \otimes \mathbb{C}^n$ and $S^{(m)}$ denotes operators which act on the Hilbert space \mathbb{C}^m .

As the spin matrices are Hermitian, trace free, 2×2 matrices, physicists often choose to multiply the previously defined $su(2)$ by i . In that case, the previously given spin matrices form a basis for $i \cdot su(2)$

$$i \cdot su(2) \equiv \left\{ \begin{pmatrix} a & c - bi \\ c + bi & -a \end{pmatrix} \mid a, b, c \in \mathbb{R} \right\}. \quad (3.10)$$

This change to the Lie algebra $su(2)$ also slightly changes its relation to the Lie group $SU(2)$. To obtain the new Lie algebra elements from the Lie group $SU(2)$ requires an additional i :

$$S_j = i \frac{\partial \hat{R}_j}{\partial \theta} \Big|_{\theta=0} \quad j = 1, 2, 3,$$

where S_j is a basis element of $i \cdot su(2)$ and \hat{R}_j is an element of $SU(2)$. Furthermore, to obtain the Lie group elements of $SU(2)$ from $i \cdot su(2)$, one has to exponentiate the

Lie algebra elements with an additional i resulting in a unitary group element. Often in quantum mechanics, the chosen convention is to also include a minus in the exponent

$$\hat{R}_j = e^{-iS_j\theta}.$$

This then results in the $SU(2)$ elements (where $\alpha = \frac{\theta}{2}$)

$$\hat{R}_x = \begin{pmatrix} \cos \alpha & -i \sin \alpha \\ -i \sin \alpha & \cos \alpha \end{pmatrix} \quad \hat{R}_y = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \quad \hat{R}_z = \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{i\alpha} \end{pmatrix}. \quad (3.11)$$

Now that we have seen that $SU(2)$ is the fundamental symmetry of non-relativistic finite-dimensional quantum systems and we have used representations of $su(2)$ to define many useful operators for modelling the spin in quantum mechanics, we can define finite-dimensional fundamental quantum systems.

Definition 8. A finite-dimensional fundamental quantum system is a quantum system whose associated Hilbert space \mathcal{H} is a finite-dimensional representation space of $SU(2)$.

In the following sections, we will consider how to decompose the state spaces of such finite-dimensional fundamental quantum systems. As this whole thesis is limited to finite-dimensional Hilbert spaces, we will always assume a quantum system is finite-dimensional in this thesis, even if this is not explicitly mentioned. An interesting result following from the fact that $SU(2)$ is the fundamental symmetry of non-relativistic quantum mechanics, is that finite-dimensional fundamental quantum systems are always invariant under a 4π ‘rotation’. Indeed, most matter that surrounds us, e.g. protons, neutrons, and electrons, is fundamentally rotation invariant under 4π and not under 2π as we so often experience. This is not just a theoretical idea but was measured in 1975 by using magnets to rotate beams of neutrons [3].

3.3 Decomposing the state spaces of fundamental quantum systems

In the first section of this chapter, we showed the inability to decompose Hilbert spaces which were composed with a tensor product and our desire to express composed Hilbert spaces as a direct sum of Hilbert spaces. Such a direct sum of Hilbert spaces could be achieved by considering the isomorphisms of composed finite-dimensional Hilbert spaces. In order to make physical sense of this decomposition and to eliminate some of the isomorphic possibilities we studied finite-dimensional fundamental quantum systems. These systems incorporate all knowledge currently available and we defined them as quantum systems whose underlying Hilbert space is a representation space of $SU(2)$. By considering the composition of fundamental quantum systems and requiring the isomorphism to again produce fundamental quantum systems, such that this direct sum decomposition must be $SU(2)$ invariant, provides a unique direct sum isomorphism.

In the first section of this chapter, we proposed to use the isomorphisms of composed Hilbert spaces as to provide a direct sum decomposition of Hilbert spaces. As this was a mathematical argument with no physical limitations we could effectively express many direct sum isomorphisms

$$\mathbb{C}^3 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \cong \mathbb{C}^7 \oplus \mathbb{C}^5 \cong \mathbb{C}^4 \oplus \mathbb{C}^3 \oplus \mathbb{C}^3 \oplus \mathbb{C}^2.$$

Now that we have defined finite-dimensional fundamental quantum systems, we require that both the composed Hilbert spaces are associated to fundamental quantum systems

as well as the Hilbert spaces in the direct sum must correspond to fundamental quantum systems. This can be achieved by finding an isomorphism of the tensor product of $SU(2)$ representation spaces that provides a direct sum of irreducible representation spaces while also being $SU(2)$ invariant. $SU(2)$ invariance implies that when we apply an element of $SU(2)$ as given in Eq.3.11 to the basis vectors of the direct sum spaces, these basis vectors must express as a linear combination of *only* basis vectors of that particular direct sum space. Such a decomposition of the Hilbert spaces of finite-dimensional fundamental quantum systems is given in the following theorem which stems from [4].

Theorem 1. For any half-integer or integer $p = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ let V_p denote a unique representation space of $su(2)$ with dimension $2p + 1$. Then for $p \geq q$

$$V_p \otimes V_q \cong V_{p+q} \oplus V_{p+q-1} \oplus \dots \oplus V_{p-q+1} \oplus V_{p-q}$$

where \cong denotes an isomorphism of $su(2)$ representations.

Proof. For a full proof see appendix A.1. □

The given vector spaces V_p in theorem 1 describe finite-dimensional representation spaces of $su(2)$. As these spaces must be the underlying Hilbert spaces for finite-dimensional fundamental quantum systems with Hilbert space $\mathcal{H} = \mathbb{C}^n$, we can use Theorem 1 and write it in a convenient form such that it is easily applicable.

Corollary 1. Let m and n be non-negative integers with $m \geq n > 0$. The composition of two fundamental quantum systems which have underlying Hilbert spaces \mathbb{C}^m and \mathbb{C}^n respectively, can be decomposed into fundamental quantum systems with the following Hilbert spaces.

$$\mathbb{C}^m \otimes \mathbb{C}^n \cong \mathbb{C}^{m+n-1} \oplus \mathbb{C}^{m+n-3} \oplus \dots \oplus \mathbb{C}^{m-n+1}.$$

Proof. The dimension of V_p as given in Theorem 1 is $2p + 1$, while the Hilbert spaces $\mathcal{H} = \mathbb{C}^m$ have dimension m . Since the Hilbert space of fundamental quantum systems must be a representation space of $su(2)$, we obtain the relation $\mathbb{C}^m = V_{\frac{1}{2}(m-1)}$. Then

$$\mathbb{C}^m \otimes \mathbb{C}^n = V_{\frac{1}{2}(m-1)} \otimes V_{\frac{1}{2}(n-1)},$$

which will have as its first subspace

$$V_{\frac{1}{2}(m-1) + \frac{1}{2}(n-1)} = V_{\frac{1}{2}(m+n)-1},$$

which has dimension $m + n - 1$ and is therefore equal to \mathbb{C}^{m+n-1} . Following Theorem 1, we can write all representation spaces in the form \mathbb{C}^p with the appropriate dimensions. □

With these results we have found a unique direct sum isomorphism that describes how to decompose the Hilbert spaces of tensor product composed finite-dimensional fundamental quantum systems. This result can be extended to the composition of multiple quantum systems as the tensor product of Hilbert spaces is associative.

3.4 Complete kinematic decomposition of quantum systems

In the previous section, we have provided a decomposition of tensor product composed $SU(2)$ representation spaces into a direct sum of irreducible representation spaces of $SU(2)$. With this knowledge, we could decompose the Hilbert spaces of finite-dimensional fundamental quantum systems into a direct sum of Hilbert spaces of finite-dimensional fundamental quantum systems. Now that we know how to decompose the Hilbert spaces, and therefore the state spaces, of composed finite-dimensional fundamental quantum systems, we want to know how to appropriately redistribute the elements of these Hilbert spaces across the direct sum Hilbert spaces. This redistribution must assign the right amount of basis vectors to each direct sum system while conserving the S_z eigenvalue of each basis eigenvector and must preserve the fundamental $SU(2)$ symmetry.

Theorem 1, by construction, provides a direct sum of representation spaces that is $SU(2)$ invariant. In other words, when an element of $SU(2)$ is applied to any basis vector of an individual direct sum Hilbert space, it will express as a linear combination of only basis vectors in that Hilbert space. Therefore, we can justify the use of direct sums as the vectors of the Hilbert spaces do not ‘mix’ and thus the Hilbert spaces are independent of each other. If v and w are each basis vectors of two different fundamental quantum systems, then $v \otimes w$ is a basis vector of their composed systems. Applying an $SU(2)$ element, \hat{R}_i with $i = 1, 2, 3$ as given in Eq.3.11, to this composed basis vector

$$R_i(v \otimes w) = (\hat{R}_i \otimes \hat{R}_i)(v \otimes w) = \hat{R}_i(v) \otimes \hat{R}_i(w),$$

will ultimately apply \hat{R}_i to the individual basis vectors, which are basis vectors of fundamental quantum systems and are therefore $SU(2)$ invariant by construction. If the decomposition provided in Theorem 1 is indeed $SU(2)$ invariant, then applying an $SU(2)$ element to basis vectors of the direct sum spaces should express as a linear combination of only basis vectors in that system. We will give a practical example to illustrate this point, from which we will find a specific change of basis that appropriately redistributes the basis vectors of the composed Hilbert spaces across the direct sum of Hilbert spaces.

Example 1. Let’s consider the decomposition of spin Hilbert spaces $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^3 \oplus \mathbb{C}$ which follows from Corollary 1. The first system is composed of two Hilbert space of dimension two, which therefore both contain an orthonormal basis of two vectors $|\frac{1}{2} \pm \frac{1}{2}\rangle$. To keep track of these vectors in this example, we will denote them by $|+\rangle = |\frac{1}{2} \frac{1}{2}\rangle$ and $|-\rangle = |\frac{1}{2} - \frac{1}{2}\rangle$. The decomposed spin systems, a spin-1 and a spin-0 system, have basis elements $|1 j\rangle$ where $j = -1, 0, 1$ and $|0 0\rangle$ respectively. Starting from the 2 level system, in the given basis we can express

$$\mathbb{C}^2 = \text{Span}_{\mathbb{C}}\{|+\rangle, |-\rangle\} \quad |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

For this example, we pick a specific $SU(2)$ element, in this case, \hat{R}_x

$$\hat{R}_x = e^{-i\theta \frac{\sigma_x}{2}} = \begin{pmatrix} \cos(\frac{\theta}{2}) & -i \sin(\frac{\theta}{2}) \\ -i \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix}.$$

If we then apply this matrix to the given basis elements, using $\alpha = \frac{\theta}{2}$ to simplify the

notation

$$\begin{aligned}\hat{R}_x|+\rangle &= \begin{pmatrix} \cos(\alpha) \\ -i \sin(\alpha) \end{pmatrix} = \cos(\alpha)|+\rangle - i \sin(\alpha)|-\rangle \\ \hat{R}_x|-\rangle &= \begin{pmatrix} -i \sin(\alpha) \\ \cos(\alpha) \end{pmatrix} = -i \sin(\alpha)|+\rangle + \cos(\alpha)|-\rangle.\end{aligned}$$

We can similarly extend this to the composed system, where without confusion we can define $|+\rangle \otimes |-\rangle = |+-\rangle$:

$$\begin{aligned}(\hat{R}_x \otimes \hat{R}_x)|++\rangle &= \cos^2(\alpha)|++\rangle - i \sin(\alpha) \cos(\alpha)(|+-\rangle + |-+\rangle) - \sin^2(\alpha)|--\rangle \\ (\hat{R}_x \otimes \hat{R}_x)|+-\rangle &= -i \sin(\alpha) \cos(\alpha)(|++\rangle + |--\rangle) + \cos^2(\alpha)|+-\rangle - \sin^2(\alpha)|-+\rangle \\ (\hat{R}_x \otimes \hat{R}_x)|-+\rangle &= -i \sin(\alpha) \cos(\alpha)(|++\rangle + |--\rangle) - \sin^2(\alpha)|+-\rangle + \cos^2(\alpha)|-+\rangle \\ (\hat{R}_x \otimes \hat{R}_x)|--\rangle &= -\sin^2(\alpha)|++\rangle - i \sin(\alpha) \cos(\alpha)(|+-\rangle + |-+\rangle) + \cos^2(\alpha)|--\rangle.\end{aligned}$$

As can be seen, applying the $SU(2)$ elements will express all basis vectors of $\mathbb{C}^2 \otimes \mathbb{C}^2$ as linear combinations of all the basis vectors of that space. If we want to redistribute these basis vectors such that in the direct sum decomposition every Hilbert space gets the appropriate amount of basis vectors equal to its dimension, while ensuring that the direct sum decomposition is $SU(2)$ invariant, we introduce the following unique change of basis

$$\begin{aligned}|11\rangle &= |++\rangle \\ |10\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \\ |1-1\rangle &= |--\rangle \\ |00\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle).\end{aligned}$$

This change of basis will express the previously given linear combinations such that the basis vectors that describe a spin-1 or spin-0 system are now expressed as a linear combination of basis vectors of their own Hilbert space.

$$\begin{aligned}\hat{R}_x|11\rangle &= \cos^2(\alpha)|11\rangle - i\sqrt{2}\sin(\alpha)\cos(\alpha)|10\rangle - \sin^2(\alpha)|1-1\rangle \\ \hat{R}_x|10\rangle &= \frac{-i\sin(2\alpha)}{\sqrt{2}}(|11\rangle + |1-1\rangle) + \cos(2\alpha)|10\rangle \\ \hat{R}_x|1-1\rangle &= -\sin^2(\alpha)|11\rangle - i\sqrt{2}\sin(\alpha)\cos(\alpha)|10\rangle + \cos^2(\alpha)|1-1\rangle \\ \hat{R}_x|00\rangle &= |00\rangle.\end{aligned}$$

Indeed, the spin-1 system with Hilbert space $\mathcal{H} = \mathbb{C}^3$, contains the vectors $|1-1\rangle, |1,0\rangle$ and $|1,1\rangle$, and when applying \hat{R}_x to any of these basis vectors will express each of them as a linear combination of only these three basis vectors. The same happens for the spin-0 system. This example only uses one of the three elements of $SU(2)$, namely \hat{R}_x , but instead applying \hat{R}_y or \hat{R}_z will yield similar results

Example 1 shows, that a decomposition as given in Corollary 1, $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^3 \oplus \mathbb{C}$, is indeed $SU(2)$ invariant, but, more importantly, we have found a unique change of basis that describes how to redistribute the vectors across the appropriate direct sum spaces while preserving their S_z eigenvalues. The change of basis chosen in example 1 is the

well known Clebsch-Gordan change of basis. It is often used in physics for combining the angular momentum and spin of multiple particles and has been studied intensively such that it is known for all possible decompositions of spin systems. In port-Hamiltonian fashion, we tried to understand the composition and decomposition of finite-dimensional fundamental quantum systems and as it turns out we require the Clebsch-Gordan change of basis to properly redistribute the Hilbert space elements of composed fundamental quantum systems. We now fully know how to express composed finite-dimensional fundamental quantum systems as a direct sum of finite-dimensional fundamental quantum system and this rightfully constitutes a kinematic decomposition. As the tensor product follows from the axioms of quantum mechanics its use is inevitable and it prevents us to look at quantum systems with a ‘classical mindset’, such that making a distinction between, for example, two separate electrons or one single system of electrons is not possible. With this kinematic decomposition, we can now again think of two separate systems as one (larger) system and vice versa. In the case of electrons, which are spin-1/2 particles similar to example one, we can not think of two electrons separate or not, but instead, we can think of a spin-1 and spin-0 particle separately.

4 Towards a dynamical decomposition of quantum systems

Now that we have provided a kinematic decomposition of finite-dimensional fundamental quantum systems, describing how to decompose Hilbert spaces and their elements, we want to describe the dynamics of fundamental quantum systems. As we considered finite-dimensional quantum systems, and therefore ignore the translational degrees of freedom, this chapter will focus on modelling the dynamics of spin systems. In this chapter, we will give a general Hamiltonian description of composed spin systems, define interaction between composed spin systems, and we will study the importance of energy degeneracy following from the conservation of energy.

4.1 Constructing the Hamiltonian of composed spin systems

In this section, we will construct the general Hamiltonian of individual as well as composed finite-dimensional quantum systems. As we only consider finite-dimensional quantum systems, we will, from now on, call them spin systems. From the composition of two spin systems, we will define interaction and model the interaction between the two systems with an interaction Hamiltonian.

The spin of a particle is proportional to a magnetic dipole moment, μ

$$\mu = \gamma S,$$

where γ is the gyromagnetic ratio. If a particle, with a magnetic moment, is then placed in a magnetic field it experiences a torque that aligns the magnetic moment parallel to the magnetic field. The energy associated to this torque is

$$H = -\vec{\mu} \cdot \vec{B},$$

where \vec{B} is the magnetic field and H the Hamiltonian. In 3d space, the Hamiltonian can be described as

$$H = -\gamma \vec{B} \cdot S = -\gamma(B_x S_x + B_y S_y + B_z S_z).$$

If we only align a magnetic field along the z direction, the Hamiltonian will be directly proportional to S_z , and similarly, the energy levels of the Hamiltonian will be directly proportional to the eigenvalues of S_z , which we called the spin levels. By assuming $\hbar = 1$ we can define $E = -\gamma B_z$ as $-\gamma B_z$ multiplied with \hbar has units of energy. This then provides a more simplified Hamiltonian

$$H = E S_z. \tag{4.1}$$

If we consider a 2 level spin system, with Hilbert space $\mathcal{H} = \mathbb{C}^2$, and describe its spin vectors as in example 1

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

then according to Eq.4.1, the top state, in this case $|+\rangle$, will correspond to an energy of $\frac{1}{2}E$ and the bottom — or often also called the ground state — will correspond to an energy of $-\frac{1}{2}E$. This interpretation is reflected in the fact that since the Hamiltonian is Hermitian,

we can reconstruct it from its from its spectral decomposition⁵

$$\begin{aligned} H_1 &= \sum_{\mathcal{E} \in \text{spec}(H_1)} \mathcal{E} P_{\mathcal{E}} = \frac{E}{2} P_{\frac{E}{2}} + \left(\frac{-E}{2}\right) P_{\frac{-E}{2}} = \frac{E}{2} |+\rangle\langle +| + \left(\frac{-E}{2}\right) |-\rangle\langle -| \\ &= \frac{E}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{E}{2} \sigma_3 = E S_z^{(1/2)}, \end{aligned}$$

which is indeed the same as the given definition for the Hamiltonian in Eq.4.1. As the Hamiltonian for spin systems is proportional to the S_z operator which is defined by a representation of $su(2)$, the Hamiltonian of a composed spin system can be described by the tensor product of $su(2)$ representations as given in definition 7. The Hamiltonian for a spin- n system coupled to a spin- m system can thus be described by

$$H_0 = H_1 \otimes I_2 + I_1 \otimes H_2 = E S_z^{(n)} \otimes I_2 + I_1 \otimes E S_z^{(m)}, \quad (4.2)$$

where H_0 denotes that this is a non-interacting Hamiltonian of a composed spin system and $S_z^{(n)}$ describes the spin operator for a spin- n particle, where in the right basis it is a diagonal matrix with eigenvalues $-n, -n+1, \dots, n-1, n$.

Now that we have coupled two spin systems and since both spin systems have evenly spaced energy gaps (between their spin levels) of the same size, we can define interaction. For interaction to take place, one of the systems must lower in energy, therefore emitting a photon, which raises the other system by exactly that amount of energy. As we have seen previously, lowering and raising the spin states, and thus effectively the energy, is done by the ladder operators as defined in Eq.3.8. As we assume that energy is conserved, the interaction term of the Hamiltonian must contain the lowering and raising operators simultaneously. We can, therefore, model this interaction with an interaction Hamiltonian of the following form

$$H_{int} = \gamma \left(S_+^{(n)} \otimes S_-^{(m)} + S_-^{(n)} \otimes S_+^{(m)} \right), \quad (4.3)$$

where γ from now on is the interaction strength (any real number) and not the gyromagnetic ratio. Since the Hamiltonian must be Hermitian, the interaction Hamiltonian must contain both possible interaction terms. The total Hamiltonian is then given as the sum of the interacting and non-interacting Hamiltonian

$$H_\gamma = H_0 + H_{int} = E S_z^{(n)} \otimes I_2 + I_1 \otimes E S_z^{(m)} + \gamma \left(S_+^{(n)} \otimes S_-^{(m)} + S_-^{(n)} \otimes S_+^{(m)} \right). \quad (4.4)$$

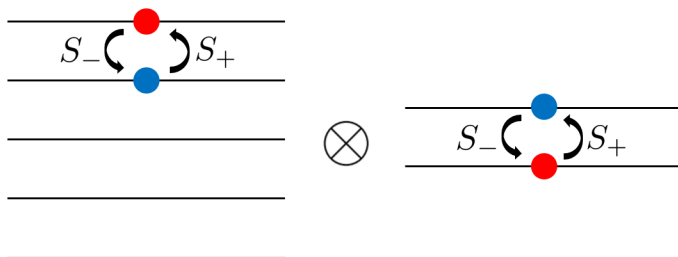


FIGURE 1: Interaction between a 5 level and 2 level spin system

⁵The eigenprojectors can be given by $|+\rangle\langle +|$ and $|-\rangle\langle -|$, where $|+\rangle\langle +|$ corresponds to the multiplication of a column vector with a row vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$.

4.2 The dynamics of spin systems

Now that we have constructed the general Hamiltonian for composed spin systems, we can find the time evolution of the quantum state that describes the system by solving the Schrödinger equation as provided in axiom 2. In this section, we will work out the quantum dynamics of the composed spin state such that we can fully describe its behaviour.

When we describe a quantum system, we can assume that we can pick any (feasible) initial conditions. Practically, this would mean we let the system evolve and measure it repeatedly, once we obtain the desired initial conditions we start our experiment. Since at no point do we not obtain the measured data, therefore not creating any classical ignorance and generating any mixed states, we can describe the system with pure states. As pure states are unique dependent on the state vectors ψ , we can work with the state vectors to describe the dynamics. To clearly illustrate the dynamics of a composed spin system we start with a spin-1/2 and a spin- m system. We again pick the orthonormal basis of the Hilbert space to be the eigenvectors of S_z such that these (spin) state vectors are also eigenvectors of the Hamiltonian. We then choose the state vectors β_b with $b = -1/2, 1/2$ for the spin-1/2 system and α_n with $n = -m, -m+1, \dots, m-1, m$ for the spin- m system⁶. As we also want to express an orthonormal basis in the composed quantum system, we naturally extend the definition of an inner product such that it can be used for tensor product composed vector spaces $\langle\langle \cdot | \cdot \rangle\rangle_{\beta \otimes \alpha} = \langle \cdot | \cdot \rangle_{\beta} \langle \cdot | \cdot \rangle_{\alpha}$. The new basis in the composed quantum system, consisting of the tensor product of the basis vectors of the individual systems, contains eigenvectors of the total non-interacting Hamiltonian

$$\begin{aligned} H_0(\beta_b \otimes \alpha_n) &= (E\sigma_z \otimes I_2 + I_1 \otimes ES_z)(\beta_b \otimes \alpha_n) = bE\beta_b \otimes \alpha_n + nE\beta_b \otimes \alpha_n \\ &= E(b+n)(\beta_b \otimes \alpha_n), \end{aligned}$$

where σ_z is the S_z operator for the two level system and S_z is the spin level operator for the spin- m system. Generally, for energy eigenvectors ψ_k where $\psi_k = \psi_{(b,n)} = \beta_b \otimes \alpha_n$, the non-interacting Hamiltonian can be written as

$$H_0\psi_k = E_k\psi_k. \quad (4.5)$$

We can describe the solutions of the non-interacting Schrödinger equation as a superposition of energy eigenvectors

$$\psi(t) = \sum_l a_l(t)\psi_l e^{-iE_l t/\hbar}, \quad (4.6)$$

where the time-dependence of the state vectors is carried by the coefficients $a_l(t)$ which describe the contribution of the respective eigenvectors to the superposition over time. These solutions can then be applied to the interacting Schrödinger equation H_γ

$$\begin{aligned} H_\gamma\psi &= \sum_l a_l(t)(H_0 + H_{int})(\psi_l e^{-iE_l t/\hbar}) \\ &= \sum_l a_l(t)e^{-iE_l t/\hbar}(E_l\psi_l + H_{int}\psi_l) \\ &= i\hbar\frac{\partial\psi}{\partial t} = \sum_l e^{-iE_l t/\hbar}\psi_l\left(i\hbar\frac{\partial a_l}{\partial t} + a_l E_l\right). \end{aligned}$$

⁶In the notation of previous chapters $\beta_{(-1/2)} = |\frac{1}{2} - \frac{1}{2}\rangle$ but in this chapter I have opted for a slightly more compact notation.

Applying $\langle \psi_k |$ to both sides of the Schrödinger equation

$$\sum_l a_l(t) e^{-iE_l t/\hbar} (E_l \delta_{kl} + \langle \psi_k | H_{int} | \psi_l \rangle) = \sum_l e^{-iE_l t/\hbar} \delta_{kl} (i\hbar \dot{a}_l + a_l E_l),$$

then results in

$$i\hbar \dot{a}_k = \sum_l a_l(t) e^{-i(E_l - E_k)t/\hbar} H'_{kl}, \quad (4.7)$$

where

$$H'_{kl} = \langle \psi_k | H_{int} | \psi_l \rangle. \quad (4.8)$$

From these differential equations it becomes evident that if there is no interaction, i.e. $\gamma = 0$, the coefficients do not depend on time, resulting in a superposition of energy eigenvectors that is stagnant. Additionally, the time-dependent coefficients, with their initial values, describe the whole dynamics of the system. To understand the full dynamics of the system the $H'_{kl} = H'_{(b,n),(b',n')}$ term must be calculated.

$$\begin{aligned} H'_{(b,n),(b',n')} &= \langle \langle \beta_b \otimes \alpha_n | H_{int} | \beta_{b'} \otimes \alpha_{n'} \rangle \rangle \\ &= \gamma \langle \langle \beta_b \otimes \alpha_n | \sigma_- \otimes S_+ + \sigma_+ \otimes S_- | \beta_{b'} \otimes \alpha_{n'} \rangle \rangle \\ &= \gamma (\langle \beta_b | \sigma_- | \beta_{b'} \rangle \langle \alpha_n | S_+ | \alpha_{n'} \rangle + \langle \beta_b | \sigma_+ | \beta_{b'} \rangle \langle \alpha_n | S_- | \alpha_{n'} \rangle) \\ &= \gamma \left(\sqrt{m(m+1) - n'(n'+1)} \delta_{n,n'+1} \delta_{b,b'-1} + \sqrt{m(m+1) - n'(n'-1)} \delta_{n,n'-1} \delta_{b,b'+1} \right), \end{aligned}$$

where σ_{\pm} denotes the ladder operators in the two level system and S_{\pm} denotes the ladder operator in the m -level system from which the square root stem as given in Eq.3.8. The ladder operators for the spin-1/2 system carry no coefficient and the other raising coefficient can be simplified by $C_m = m(m+1)$. The dynamics of the system are then described by Eq.4.7 and since the spin-1/2 system consists of only two levels $b = -1/2, 1/2$ it can be written out explicitly⁷

$$\begin{aligned} i\dot{a}_{(1/2,n)} &= \sum_{b' \in \{-1/2, 1/2\}} \sum_{n'=-m}^m a_{(b',n')}(t) e^{-i(E_{(b',n')} - E_{(1/2,n)})t} \\ &\quad \gamma \left(\sqrt{C_m - n'(n'+1)} \delta_{n,n'+1} \delta_{1/2,b'-1} + \sqrt{C_m - n'(n'-1)} \delta_{n,n'-1} \delta_{1/2,b'+1} \right) \\ &= \gamma \sqrt{C_m - n(n+1)} a_{(-1/2,n+1)} \\ i\dot{a}_{(-1/2,n)} &= \sum_{b' \in \{-1/2, 1/2\}} \sum_{n'=-m}^m a_{(b',n')}(t) e^{-i(E_{(b',n')} - E_{(-1/2,n)})t} \\ &\quad \gamma \left(\sqrt{C_m - n'(n'+1)} \delta_{n,n'+1} \delta_{-1/2,b'-1} + \sqrt{C_m - n'(n'-1)} \delta_{n,n'-1} \delta_{-1/2,b'+1} \right) \\ &= \gamma \sqrt{C_m - n(n-1)} a_{(1/2,n-1)}, \end{aligned}$$

where we used the degeneracy in the energy $E(-1/2, n+1) = E(1/2, n) = (n+1/2)E$. This energy degeneracy is expected as energy conservation only allows these two energy levels to interact with each other. It is also important to note that these are coupled first order differential equations, the time derivative of a coefficient is dependent on the

⁷For most practical purposes we will assume $\hbar = 1$.

coefficient of its degenerate partner state

$$\begin{aligned}
\dot{a}_{(1/2,n)} &= -i\gamma\sqrt{C_m - n(n+1)} a_{(-1/2,n+1)} \\
\dot{a}_{(-1/2,n+1)} &= -i\gamma\sqrt{C_m - n(n+1)} a_{(1/2,n)} \\
\dot{a}_{(1/2,m)} &= 0 \\
\dot{a}_{(-1/2,-m)} &= 0.
\end{aligned} \tag{4.9}$$

The last line shows that the states $|-\rangle \otimes |-m\rangle$ and $|+\rangle \otimes |m\rangle$ are time-independent, which makes sense as these are the ground state and top state of the composed system. From this example, it becomes clear that energy degeneracy is indeed necessary for interaction if we want to respect energy conservation. Both the top and ground states have energy degeneracy one, and thus will not interact. The first order coupled differential equations can be linked to get two second order (uncoupled) differential equations

$$\begin{aligned}
\ddot{a}_{(-1/2,n+1)} &= -\left(\gamma\sqrt{C_m - n(n+1)}\right)^2 a_{(-1/2,n+1)} \\
\ddot{a}_{(1/2,n)} &= -\left(\gamma\sqrt{C_m - n(n+1)}\right)^2 a_{(1/2,n)},
\end{aligned} \tag{4.10}$$

which are the famous harmonic oscillator differential equations. Solving the ODE's results in

$$\begin{aligned}
a_{(-1/2,n+1)}(t) &= \frac{1}{2} \left(a_{(-1/2,n+1)}(0) - a_{(1/2,n)}(0) \right) e^{i\gamma\sqrt{C_m - n(n+1)}t} \\
&\quad + \frac{1}{2} \left(a_{(-1/2,n+1)}(0) + a_{(1/2,n)}(0) \right) e^{-i\gamma\sqrt{C_m - n(n+1)}t} \\
a_{(1/2,n)}(t) &= -\frac{1}{2} \left(a_{(-1/2,n+1)}(0) - a_{(1/2,n)}(0) \right) e^{i\gamma\sqrt{C_m - n(n+1)}t} \\
&\quad + \frac{1}{2} \left(a_{(-1/2,n+1)}(0) + a_{(1/2,n)}(0) \right) e^{-i\gamma\sqrt{C_m - n(n+1)}t}.
\end{aligned}$$

Now that we have completely solved the differential equations that described the dynamics of the statevector, we can completely describe it as described in Eq.4.7

$$\begin{aligned}
\psi(t) &= a_{(-1/2,-m)}\beta_{-1/2} \otimes \alpha_{-m} e^{i(\frac{1}{2}+m)Et} + a_{(1/2,m)}\beta_{1/2} \otimes \alpha_m e^{-i(\frac{1}{2}+m)Et} \\
&\quad + \sum_{n=-m}^{m-1} a_{(-1/2,n+1)}(0) \left(\cos(\gamma At)\beta_{-1/2} \otimes \alpha_{n+1} - i \sin(\gamma At)\beta_{1/2} \otimes \alpha_n \right) e^{-iE(n+\frac{1}{2})t} \\
&\quad + \sum_{n=-m}^{m-1} a_{(1/2,n)}(0) \left(-i \sin(\gamma At)\beta_{-1/2} \otimes \alpha_{n+1} + \cos(\gamma At)\beta_{1/2} \otimes \alpha_n \right) e^{-iE(n+\frac{1}{2})t},
\end{aligned}$$

where $A = \sqrt{C_m - n(n+1)}$ to make everything a bit more compact. This is a complete solution to the interacting Schrödinger equation. Given initial conditions, we can fully describe $\psi(t)$ and how it behaves with time. Since we are still working with a pure state, we can describe the state $\rho = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$ from the given initial conditions. This example is not completely general as I wanted to give a clear and in depth description of dynamics of coupled spin systems. By using a 2-level spin system, as the energy degeneracy is limited to the smallest composed spin system, we could write out the dynamical equations explicitly which gave a lot of insight into this interaction. Of course, a general description of spin systems is almost similar to the description provided in this section except there will be multiple coupled first-order differential equations and the complete solution can not be written out explicitly.

4.3 The role of energy degeneracy

In the previous chapter, it became evident why the degeneracy of eigenvalues of the S_z operator was so important for the structure of decomposing fundamental quantum systems. In the previous section, interaction was only possible due to degenerate energy eigenvectors as a result of the conservation of energy. In this section, we investigate this underlying energy structure and incorporate this knowledge into a theorem, which hints at a ‘puzzle piece’ for a port-Hamiltonian description of quantum mechanics.

In the last chapter, we realized that we can decompose $su(2)$ representation spaces, that were originally composed with a tensor product, based on degenerate eigenvectors of the composed spin operator S_z . Since the energy of a spin state is directly proportional to its eigenvalue of S_z , Eq.4.1, the degenerate energy structure of the eigenvalues of the Hamiltonian is to be expected. In the previous section, we observed that by assuming energy conservation while modelling the composed spin systems, interaction can only occur if there exist degenerate energy eigenvectors. In other words, there need to be multiple eigenvectors of equal energy for the system to be capable of energy transfer from one state to another. This is illustrated by last section’s example where the top and ground states did not interact and were ‘static’. Since this degenerate behaviour is so important for interaction, it might be interesting to only consider the degenerate energy eigenspaces of the Hamiltonian.

If $[A, B] = 0$ and A has eigenvalue λ such that $Av = \lambda v$ and B has eigenvalue μ such that $Bw = \mu w$ then

$$0 = [A, B]v = ABv - BAv = A(Bv) - \lambda(Bv)$$

and therefore Bv is also an eigenvector of A with eigenvalue λ . Consequently, if $[H_0, H_{int}] = 0$ then for $v \in E_\lambda(H_0)$ the λ -energy eigenspace of H_0

$$H_{int}v \in E_\lambda(H_0), \quad H_{int}(E_\lambda(H_0)) \subseteq E_\lambda(H_0). \quad (4.11)$$

So applying the interaction Hamiltonian does not get you out of the energy eigenspace of H_0 , once they commute. Note that this is a beautiful reformulation of energy conservation. As long as the interaction Hamiltonian and the non-interaction Hamiltonian commute, interaction will not change the energy eigenspace and thus the energy before, during and after interaction will remain the same. Given a Hamiltonian we can pick an orthonormal eigenbasis $v_\lambda \in E_\lambda(H_0)$ such that

$$\mathcal{H} = \bigoplus_{\lambda \in \text{Spec}(H_0)} E_\lambda(H_0) \quad \text{and} \quad v = \sum_{\lambda \in \text{Spec}(H_0)} v_\lambda, \quad \forall v \in \mathcal{H}.$$

This then leads to the previous idea of describing the Hamiltonian of a system by its energy eigenspaces, especially since

$$\begin{aligned} (H_0 + H_{int})(E_\lambda(H_0)) &= H_0(E_\lambda(H_0)) + H_{int}(E_\lambda(H_0)) \\ &\subseteq E_\lambda(H_0) + E_\lambda(H_0) = E_\lambda(H_0), \end{aligned}$$

where we used that $H_0(E_\lambda(H_0)) = E_\lambda(H_0)$ and $[H_0, H_{int}] = 0$ which then implies Eq 4.11.

Lemma 2. Given a non-interacting Hamiltonian H_0 and an interacting Hamiltonian H_{int} . If they commute, $[H_0, H_{int}] = 0$, the following result holds

$$H_0 + H_{int} = \bigoplus_{\lambda \in \text{Spec}(H_0)} H^\lambda,$$

where

$$H^\lambda v = \begin{cases} (H_0 + H_{int})v, & v \in E_\lambda(H_0) \\ 0 & \text{else} \end{cases}$$

Proof. Using $v = \sum_\lambda v_\lambda$ for $v_\lambda \in E_\lambda(H_0)$

$$\begin{aligned} \bigoplus_\lambda H^\lambda(v) &= \bigoplus_\lambda H^\lambda \left(\sum_\mu v_\mu \right) = \sum_\lambda \sum_\mu H^\lambda(v_\mu) \\ &= \sum_\lambda \sum_\mu \delta_{\mu,\lambda} H^\lambda v_\mu = \sum_\lambda H^\lambda v_\lambda \\ &= (H_0 + H_{int}) \left(\sum_\lambda v_\lambda \right) = (H_0 + H_{int})v \end{aligned}$$

where $\delta_{\mu,\lambda}$ is the Kronecker-delta. □

Lemma 2 shows that instead of using the Hamiltonian on the entire Hilbert space we can use the Hamiltonian for each energy eigenspace separately. This only holds for $[H_0, H_{int}] = 0$, but conveniently, it turns out this is the case for all composed spin systems.

Lemma 3. For a system composed of two spin systems, a spin- n and a spin- m system, where the Hamiltonian's are given by

$$\begin{aligned} H_0 &= E \left(S_z^{(m)} \otimes I_n + I_m \otimes S_z^{(n)} \right) \\ H_{int} &= \gamma \left(S_+^{(m)} \otimes S_-^{(n)} + S_-^{(m)} \otimes S_+^{(n)} \right), \end{aligned}$$

the Hamiltonian's always commute $[H_0, H_{int}] = 0$.

Proof. Using the relations for the ladder operators $S_\pm = S_x \pm iS_y$ and that the tensor product is bilinear, H_{int} can be written as

$$H_{int} = 2\gamma \left(S_+^{(m)} \otimes S_+^{(n)} + S_y^{(m)} \otimes S_y^{(n)} \right).$$

The commutation of H_0 and H_{int} then results in

$$\begin{aligned} [H_0, H_{int}] &= 2E\gamma \left(S_x^{(m)} \otimes [S_z^{(n)}, S_x^{(n)}] + [S_z^{(m)}, S_x^{(m)}] \otimes S_x^{(n)} \right. \\ &\quad \left. + S_y^{(m)} \otimes [S_z^{(n)}, S_y^{(n)}] + [S_z^{(m)}, S_y^{(m)}] \otimes S_y^{(n)} \right). \end{aligned}$$

Using the commutation relations $[S_i, S_j] = i\varepsilon_{ijk}S_k$ the result is $[H_0, H_{int}] = 0$. □

This is a convenient result, when working with composed spin systems we know that the interaction will always conserve energy and we can work with the energy eigenspaces on at a time instead of working with the whole Hilbert space. Many of these useful properties can be combined and are encapsulated in a single theorem⁸.

Theorem 2. If $H_\gamma = H_0 + H_{int}$ with $[H_0, H_{int}] = 0$ and $i\dot{\rho} = [H_\gamma, \rho]$ where ρ is a pure state. Then

$$\text{tr}(\dot{\rho}P_{E_\lambda}(H_0)) = 0 \quad \forall \lambda \in \text{Spec}(H_0)$$

⁸The form and relevance of this theorem has been conceived together with my fellow student Kia Romero Hojjati.

Proof. For a full proof see appendix A.2. □

This seems like a very simple result, but it includes many of the properties we discovered in this section. The proof uses the energy conservation property $H_{int}(E_\lambda(H_0)) \subseteq E_\lambda(H_0)$ as it labels vectors by their energy eigenspace. In chapter 2, we saw that the probability of the system being in a certain state for a given energy is given by $P(E|\rho) = \text{tr}(\rho P_E)$, which if all degenerate energy eigenvectors are taken into account by multiple eigenprojectors, should be equal to 1. Therefore, taking the time derivative of this probability gives $\text{tr}(\dot{\rho} P_E)$. In addition to that, the trace as given in Theorem 2, contains the full dynamics of the system as given by the Schrödinger equation. Ultimately, these three properties make theorem 2 an extremely useful component as it describes the full dynamics as well as the degenerate energy structure. This might be a useful tool for constructing a port-Hamiltonian theory of quantum mechanics.

5 Conclusions

Starting with an axiomatic review of quantum mechanics, we identified the main problem for constructing a port-Hamiltonian theory of quantum mechanics. As described in the fourth axiom, the composition of quantum systems occurs by composing their Hilbert spaces with a tensor product. The existence of entangled states, which results from the increase of the dimension of the composed system, eliminates the possibility to split two Hilbert spaces composed with a tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ back into the original \mathcal{H}_1 and \mathcal{H}_2 .

In chapter 3, we realized that this problem could be circumvented if we could express the composed Hilbert spaces as a direct sum of Hilbert spaces, which by definition, would be independent of each other. In that case, an entangled state would express as a linear combination of vectors in different direct sum spaces, which could easily be separated. By considering only finite-dimensional quantum systems with Hilbert space $\mathcal{H} = \mathbb{C}^m$ we could express the isomorphisms of composed Hilbert spaces as such a desired direct sum of Hilbert spaces. Such a direct sum decomposition, however, was not unique as it was purely based on mathematical reasoning and did not take any of the physical arguments into account.

To make sure we had all the physical information to justify specific configurations of the Hilbert space isomorphisms we required only considering fundamental quantum systems. Fundamentally modelling a quantum system requires using all knowledge of quantum systems currently available without simplifying any information. We realized that $SU(2)$ is the fundamental symmetry of non-relativistic quantum mechanics and that finite-dimensional fundamental quantum systems, those with no translational degrees of freedom, must have Hilbert spaces that are representation spaces of $SU(2)$. A consequence of the fundamental $SU(2)$ symmetry is that most quantum matter around us is fundamentally rotation invariant under 4π .

By now only considering the composition of finite-dimensional fundamental quantum systems and only isomorphisms that include a direct sum of finite-dimensional fundamental quantum systems we obtained a unique isomorphism

$$\mathbb{C}^m \otimes \mathbb{C}^n \cong \mathbb{C}^{m+n-1} \oplus \mathbb{C}^{m+n-3} \oplus \dots \oplus \mathbb{C}^{m-n+1}$$

that respects the fundamental $SU(2)$ symmetry of non-relativistic quantum mechanics. Although the axioms of quantum mechanics require us to compose quantum systems with a tensor product, now there do exist certain quantum systems that can be composed with a direct sum as long as they correspond to a possible tensor product composition. This classical way of thinking now allows us to consider, for example, two electrons, which are spin-1/2 particles, as one spin-1 particle *and* one spin-0 particle.

Although we had found a way to decompose the Hilbert spaces of finite-dimensional fundamental quantum systems, we still had to find a change of basis such that the elements of these systems were redistributed appropriately. We found that the unique Clebsch-Gordan change of basis preserves the $SU(2)$ invariance in the direct sum decomposition, provides a basis for each direct sum system and conserves the eigenvalues of S_z for each basis vector. Therefore, we have provided a complete description of the decomposition of finite-dimensional fundamental quantum systems, describing how to decompose both the Hilbert spaces as well as their elements, and this rightfully constitutes a ‘kinematic decomposition of finite-dimensional fundamental quantum systems’.

Although this kinematic decomposition is the main result of this thesis, a first attempt at a dynamic decomposition of quantum systems was made. The Hamiltonian and the full dynamics of composed spin systems were derived. Due to energy conservation, only

interaction between degenerate energy eigenstates was possible. We then realized that if the interacting and non-interacting Hamiltonian's commute we could analyze the system by looking at the specific energy eigenspaces instead of looking at the whole Hilbert space at once. As much of the dynamical structure is a consequence of this energy degeneracy, this approach makes the dynamics much more transparent and will help a lot in future attempts of finding a complete dynamical decomposition.

Much work has been done on trying to understand the dynamics in the direct sum decomposition. Unfortunately, due to time limitations, not enough concrete results have been obtained to mention in this thesis. It does, however, seem that most physical components can be carried to the direct sum decomposed systems by the simple transformation $A_{\oplus} = TA_{\otimes}T^{-1}$, where the transformation T is the described Clebsch-Gordan change of basis. Even Theorem 2 conveniently seems to apply in the direct sum system. This makes future research into the dynamical decomposition much more pleasant as then the dynamics can be described by only regarding the individual energy eigenspaces.

This research has been done with the greater purpose of constructing a port-Hamiltonian theory of quantum mechanics. Although not explained here, it aims at describing open quantum systems and how they are connected such that the overall energy is preserved and the full dynamics of the system are described. Such a theory would give a rigorous description of a theory of interaction within quantum mechanics. A major goal of this research was to find the power ports, which exist in classical port-Hamiltonian theory. This has not been accomplished yet but with the kinematic decomposition that was described in this thesis, a dynamic decomposition seems insight.

This research was limited to finite-dimensional quantum systems, as one only needed to have knowledge of linear algebra. Additionally, we modelled all quantum systems as fundamental quantum systems, describing all details and no effective models. The ultimate goal is to make a port-Hamiltonian description of most physical theories that can be formulated in a Hamiltonian fashion. For non-relativistic quantum mechanics, the fundamental symmetry group is $SU(2)$. If a complete port-Hamiltonian theory of non-relativistic quantum mechanics was formulated this could possibly be extended to relativistic quantum theory by changing the symmetry group to $sl(2, \mathbb{C})$, as its representations describe relativistic spin. It could be that by formulating a rigorous theory of interactions of quantum mechanics it would be relatively simple to extend this idea to more areas of physics.

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A Appendix

A.1 Proof of Theorem 1

The original proof of this theorem comes from [4]. I modified it slightly but it is still the same proof.

Proof. Take a basis for each of the two spaces V_m and V_n and label them by their eigenvalues of S_z , the spin levels. So we get the bases $u_m, u_{m-1}, \dots, u_{-m}$ for V_m and $v_n, v_{n-1}, \dots, v_{-n}$ for V_n . As these are eigenvectors of S_z for their respective space $S_z u_m = m u_m$ and $S_z v_n = n v_n$. Then the composed vectors $u_i \otimes v_j$ form a basis for $V_m \otimes V_n$ such that if S_z is applied to the composed system⁹

$$\left(S_z^{(m)} \otimes I + I \otimes S_z^{(n)} \right) u_i \otimes v_j = (i + j) u_i \otimes v_j.$$

Thus each basis element is an eigenvector of S_z on $V_m \otimes V_n$, with eigenvalues ranging from $m + n$ to $-(m + n)$ in increments of 1. The eigenspace with eigenvalue $m + n$, the largest eigenvalue, is one dimensional and is spanned by $u_m \otimes v_n$. If $n > 0$, i.e. the second space has dimension higher than 1, then the eigenspace with eigenvalue $m + n - 1$ has dimension 2 and is spanned by $u_{m-1} \otimes v_n$ and $u_m \otimes v_{n-1}$. Each time we decrease the eigenvalue of S_z by one, we increase the degeneracy of the corresponding eigenspace by 1. This continues until we reach the eigenvalue $m - n$, an eigenvalue with max degeneracy, with an eigenspace spanned by

$$u_m \otimes v_{-n}, u_{m-1} \otimes v_{-n+1}, \dots, u_{m-2n+1} \otimes v_{n-1}, u_{m-2n} \otimes v_n.$$

This space has dimension $2n + 1$. If we continue decreasing the eigenvalue of S_z by one in each step, the dimension remains the same until we reach the eigenvalue $n - m$. After this eigenvalue, the dimension of the eigenspace starts to decrease by one, similar to the structure of the top eigenvalues. This continues until we reach the lowest eigenvalue $-(m + n)$ which has an eigenspace of dimension 1 and is spanned by $u_{-m} \otimes u_{-n}$. This pattern is illustrated in the following table for V_2 , with dimension 5, and V_1 with dimension 3. The total dimension of the composed system is 15 and thus we get the following 15 basis vectors.

Eigenvalues for S_z	Basis		
3	$u_2 \otimes v_1$		
2	$u_1 \otimes v_1$	$u_2 \otimes v_0$	
1	$u_0 \otimes v_1$	$u_1 \otimes v_0$	$u_2 \otimes v_{-1}$
0	$u_{-1} \otimes v_1$	$u_0 \otimes v_0$	$u_1 \otimes v_{-1}$
-1	$u_{-2} \otimes v_1$	$u_{-1} \otimes v_0$	$u_0 \otimes v_{-1}$
-2	$u_{-2} \otimes v_0$	$u_{-1} \otimes v_{-1}$	
-3	$u_{-2} \otimes v_{-1}$		

In the general case, consider the first eigenvector $u_m \otimes v_n$ with the largest eigenvalue for S_z of $m + n$. It is annihilated by S_+ as it is the top spin level. We can lower the spin level by S_- and applying the operator repeatedly gives a chain of eigenvectors for S_z with eigenvalues lowered by one until they reach $-(m + n)$. We define the span of these vectors, as W , which is invariant under $su(2)$ as if we apply any of the basis elements of $su(2)$, S_+, S_-, S_z , we still get an element in W . Therefore by linear extension, any element of $su(2)$ applied to W will give us an element of W . According to [4], the span of W is also irreducible and isomorphic to V_{m+n} as W contains $2(m + n) + 1$ vectors. Additionally, the orthogonal

⁹From now on we will define S_z, S_+, S_- as in Eq.3.9 for composed systems.

complement of W is also invariant under actions of $su(2)$. Since W contains eigenvectors for all eigenvalues of S_z with multiplicity one, each eigenvector for S_z in W^\perp will have its multiplicity lowered by one. As the top and bottom spin level only had multiplicity 1 and are part of W , the highest eigenvalue of W^\perp will be one lower than that of W . So $m+n$ is not an eigenvalue of S_z in W^\perp but the largest eigenvalue in W^\perp is $m+n-1$ with multiplicity one.

Now if we start at the top eigenvector for S_z in W^\perp , so with eigenvalue $m+n-1$, it will be annihilated by S_+ in W^\perp . We can apply the lowering operator to again gain a string of eigenvectors, this time of length $2(m+n)+1-2=2(m+n-1)+1$. Therefore this process generates an irreducible invariant subspace isomorphic to V_{m+n-1} .

We then repeat this process, at each step looking at the orthogonal complement of the sum of all invariant subspaces that we have obtained in previous stages. Each step reduces the multiplicity of the S_z -eigenvalue by 1 and thereby reduces the largest remaining eigenvalue of S_z by one. This process can continue until all degenerate eigenvectors are in a different irreducible subspace. As the maximum degeneracy of $V_m \otimes V_n$ is $2n+1$ and every new subspace has a dimension of 2 lower than the previous subspace, starting with dimension $2(m+n)+1$ we end with dimension $2(m+n)+1-4n=2(m-n)+1$. Thus the last subspace will be V_{m-n} . \square

A.2 Proof of Theorem 2

In this section, I will first state Theorem 2, then give the idea behind the proof and then give the actual proof.

Theorem. If $H_\gamma = H_0 + H_{int}$ with $[H_0, H_{int}] = 0$ and $i\dot{\rho} = [H, \rho]$ where ρ is a pure state. Then

$$tr(\dot{\rho} P_{E_\lambda}(H_0)) = 0 \quad \forall \lambda \in Spec(H_0).$$

The idea of the proof is very similar to the derivation in the section 'The dynamics of spin systems'. This is a very common way to describe the quantum dynamics of a system. Using the required commutation relation given by the Theorem, we can address each energy eigenspace separately. With these properties we can proof the result. As in the proof we need to keep track of the energy eigenspaces and the orthonormal basis of that particular energy eigenspace we will label everything with two indices.

Proof. Let ρ be a pure state $\rho = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$ where $\psi(t)$ is a general solution to the Schrödinger equation for H_0 . Such a solution is of the form

$$\psi(t) = \sum_n \hat{a}_n(t) \hat{\psi}_n e^{-iE_n t/\hbar},$$

where we use hats to denote vectors containing an orthonormal basis within a specific energy eigenspace of value k .

$$\begin{aligned} \hat{\psi}_k &:= (\psi_k^{(1)}, \psi_k^{(2)}, \dots, \psi_k^{(deg(\lambda_k))}) \\ \hat{a}_k &:= (a_k^{(1)}, a_k^{(2)}, \dots, a_k^{(deg(\lambda_k))}), \end{aligned}$$

where $deg(\lambda_k)$ is the degeneracy of the energy eigenvalue. Then

$$\hat{\psi}_k \hat{a}_k = \hat{a}_k \hat{\psi}_k = \sum_{i=1}^{deg(\lambda_k)} a_k^{(i)} \psi_k^{(i)} \quad \text{and} \quad \frac{d}{dt} \hat{a}_k \hat{\psi}_k = \sum_{i=1}^{deg(\lambda_k)} \dot{a}_k^{(i)}(t) \psi_k^{(i)}.$$

Using the Schrödinger equation ($\hbar = 1$), $i\partial_t\psi = H_\gamma\psi$

$$\begin{aligned} i\partial_t\psi &= i\sum_n \dot{\hat{a}}_n(t)\hat{\psi}_n e^{-iE_n t} + i\sum_n \hat{a}_n(t)\hat{\psi}_n (-iE_n) e^{-iE_n t} \\ &= \sum_n \left(i\dot{\hat{a}}_n\hat{\psi}_n e^{-iE_n t} + \hat{a}_n\hat{\psi}_n E_n e^{-iE_n t} \right) \\ &= \sum_n e^{-iE_n t}\hat{\psi}_n \left(i\dot{\hat{a}}_n + \hat{a}_n E_n \right). \end{aligned}$$

Since $H_\gamma = H_0 + H_{int}$

$$\begin{aligned} H_\gamma\psi &= \sum_n H_0 \left(\hat{a}_n\hat{\psi}_n e^{-iE_n t} \right) + \sum_n H_{int} \left(\hat{a}_n\hat{\psi}_n e^{-iE_n t} \right) \\ &= \sum_n \hat{a}_n e^{-iE_n t} \left(H_0\hat{\psi}_n + H_{int}\hat{\psi}_n \right) \\ &= \sum_n \hat{a}_n e^{-iE_n t} \left(E_n\hat{\psi}_n + H_{int}\hat{\psi}_n \right). \end{aligned}$$

As we are working with an orthonormal basis

$$\begin{aligned} \langle \hat{\psi}_k | \hat{\psi}_n \rangle &:= \left(\langle \psi_k^{(i)} | \psi_n^{(j)} \rangle \right)_{1 \leq i \leq \deg(\lambda_k), 1 \leq j \leq \deg(\lambda_n)} \\ &= \delta_{kn} := \begin{cases} id_{E_{\lambda_n}}, & n = k \\ 0 \in \mathcal{L}(E_n, E_k), & n \neq k \end{cases} \end{aligned}$$

By then equating both sides and applying $\langle \hat{\psi}_k |$ to both sides

$$\sum_n \hat{a}_n e^{-iE_n t} (E_n \delta_{kn} + H'_{kn}) = \sum_n e^{-iE_n t} \delta_{kn} (i\dot{\hat{a}}_n + E_n \hat{a}_n).$$

Where we defined H'_{kn} in terms of the basis elements, of the two energy eigenspaces

$$H'_{kn} = \langle \hat{\psi}_k | H_{int} | \hat{\psi}_n \rangle := \left(\langle \psi_k^{(i)} | H_{int} | \psi_n^{(j)} \rangle \right)_{ij}.$$

After rewriting we end up with

$$i\dot{\hat{a}}_k = \sum_n \hat{a}_n e^{-i(E_n - E_k)t} H'_{kn}.$$

Since $H_{int}\hat{\psi}_n \in E_{\lambda_n}$ and we have an orthonormal basis

$$H'_{kk} = \delta_{kn} H'_{kn}.$$

Hence,

$$i\dot{\hat{a}}_k = H'_{kk} \hat{a}_k.$$

As ψ was previously given by a superposition, we can now write it out explicitly.

$$\begin{aligned} |\psi(t)\rangle &= \sum_n \sum_{s=1}^{\deg(\lambda_n)} e^{-iE_n t} a_n^{(s)} \left| \psi_n^{(s)} \right\rangle \\ \langle \psi(t) | &= \sum_k \sum_{j=1}^{\deg(\lambda_k)} e^{iE_k t} a_k^{*(j)} \left\langle \psi_k^{(j)} \right|. \end{aligned}$$

For example, in the composition of a two level spin system with another spin system it would look like

$$|\psi(t)\rangle = \sum_n e^{-iE(n+\frac{1}{2})t} (a_{(1/2,n)} (\beta_{1/2} \otimes \alpha_n) + a_{(-1/2,n+1)} (\beta_{-1/2} \otimes \alpha_{n+1})).$$

Combining the two expressions for the state vector

$$|\psi(t)\rangle\langle\psi(t)| = \sum_{k,n} \sum_{s,j} e^{-i(E_n - E_k)t} a_n^{(s)} a_k^{*(j)} |\psi_n^{(s)}\rangle\langle\psi_k^{(j)}|.$$

we then define the projector to the energy-eigenspace of λ_l by its eigenvector basis elements

$$P_{\mathcal{E}_l} := \sum_{m=1}^{deg(\lambda_l)} |\psi_l^{(m)}\rangle\langle\psi_l^{(m)}|.$$

Applying the projector

$$\begin{aligned} |\psi(t)\rangle\langle\psi(t)|P_{\mathcal{E}_l} &= \sum_{k,n} e^{-i(E_n - E_k)t} |\hat{a}_n \hat{\psi}_n\rangle\langle\hat{a}_k \hat{\psi}_l| \delta_{k,l} \\ &= \sum_n e^{-i(E_n - E_l)t} |\hat{a}_n \hat{\psi}_n\rangle\langle\hat{a}_l \hat{\psi}_l|. \end{aligned}$$

Since unitary time evolution preserves the inner product $\langle\psi(0)|\psi(0)\rangle = \langle U(t)\psi(0)|U(t)\psi(0)\rangle = \langle\psi(t)|\psi(t)\rangle$ the probability of measuring energy $\mathcal{E} = lE$ is given by:

$$p(\mathcal{E} = lE|\rho) = tr(\rho P_{\mathcal{E}_l}) = \frac{1}{\langle\psi(0)|\psi(0)\rangle} \sum_n e^{-i(E_n - E_l)t} tr(|\hat{a}_n \hat{\psi}_n\rangle\langle\hat{a}_l \hat{\psi}_l|).$$

Since

$$\begin{aligned} tr(|\hat{a}_n \hat{\psi}_n\rangle\langle\hat{a}_l \hat{\psi}_l|) &= \sum_{i,j} a_n^{(i)} a_l^{*(j)} tr(|\psi_n^{(i)}\rangle\langle\psi_l^{(j)}|) \\ &= \sum_{i,j} \delta_{n,l} \delta_{i,j} a_n^{(i)} a_l^{*(j)} = \sum_i |a_l^{(i)}|^2. \end{aligned}$$

Thus

$$p(\mathcal{E} = lE|\rho) = tr(\rho P_{\mathcal{E}_l}) = \frac{1}{\langle\psi(0)|\psi(0)\rangle} \sum_i^{deg(\lambda_l)} |a_l^{(i)}(t)|^2.$$

Now that we know the above given relation holds we can look at the summand

$$\begin{aligned} tr(\rho P_{\mathcal{E}_l}) = 0 &\iff \|\hat{a}_l\|^2 = 0 \\ tr(\dot{\rho} P_{\mathcal{E}_l}) = 0 &\iff \frac{d}{dt} \|\hat{a}_l\|^2 = 0. \end{aligned}$$

Continuing with the norm squared approach

$$\frac{d}{dt} \|\hat{a}_l\|^2 = \frac{d}{dt} \left(\sum_{i=1}^{deg(\lambda_l)} a_l^{(i)} a_l^{*(i)} \right) = \sum_i \dot{a}_l^{(i)} a_l^{*(i)} + a_l^{(i)} \dot{a}_l^{*(i)}.$$

Substituting the previously found equation, $i\dot{a}_k^{(j)} = \sum_i H_{ji}^k a_k^{(i)}$, for the time derivatives of the coefficients

$$\begin{aligned}
\frac{d}{dt} \|\hat{a}_l\|^2 &= \frac{d}{dt} \left(\sum_j a_l^{(j)} a_l^{*(j)} \right) = \sum_j \dot{a}_l^{(j)} a_l^{*(j)} + a_l^{(j)} \dot{a}_l^{*(j)} \\
&= \sum_j \left\{ \left(-i \sum_p H_{jp}^l a_l^{(p)} \right) a_l^{*(j)} + a_l^{(j)} \left(i \sum_q H_{jq}^{*l} a_l^{*(q)} \right) \right\} \\
&= i \sum_j \left\{ \sum_q H_{jq}^{*l} a_l^{(j)} a_l^{*(q)} - \sum_p H_{jp}^l a_l^{(p)} a_l^{*(j)} \right\} \\
&= i \left\{ \sum_{j,q} H_{jq}^l a_l^{(j)} a_l^{*(q)} - \sum_{j,p} H_{jp}^l a_l^{(p)} a_l^{*(j)} \right\} = 0.
\end{aligned}$$

Where we used that the Hamiltonian is Hermitian and thus taking the complex conjugate with the star results in $H_{ab}^* = H_{ba}$. \square