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Nonlinear models: from Quantum Biology to Quantum Hybrids

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Contents

Introduction

This thesis aims to explore two relevant topics in the field of quantum physics and applied mathematics: quantum hybrid systems and excitation energy transfer in photosynthetic complexes. Although seemingly distinct, these subjects share a common thread involving the application of quantum dynamics in complex physical and biological contexts. Classical physics has provided a solid foundation for understanding numerous natural phenomena. However, as we delve deeper into the study of complex biological systems and novel quantum technologies, it becomes evident that classical models are insufficient to fully explain certain processes.
On a microscopic scale, quantum phenomena cannot be neglected. In fact, in spectroscopy devices [35], it became necessary to employ models based on mathematical tools typical of quantum mechanics [34].
In emerging technologies, such as atomtronics, the quantum models analyzed in this thesis represent an interaction modelization. Atomtronics [1] is an emerging field of physics that focuses on the creation of circuits, devices, and systems using ultra-cold atoms, typically confined and manipulated within optical or magnetic potentials on branched manifolds. Atomtronics heavily relies on Bose-Einstein condensates (BECs) and ultra-cold Fermi gases. These systems exhibit quantum behavior at macroscopic scales, such as superfluidity, coherence, and collective excitations.
Biological systems, particularly those involved in processes such as neural activity, vision, and olfaction, exhibit extraordinary performance that current classical theories do not explain.

Part I of the thesis broadens the exploration of stationary solutions to nonlinear Schrödinger equations within quantum hybrid systems. Quantum hybrid systems are multidimensional structures in which quantum dynamics is defined on manifolds of different dimensions that are connected in such a way that a nontrivial dynamics is established on the entire structure. The core of this research focuses on the analysis of stationary solutions for the nonlinear Schrödinger equations on quantum hybrids, with particular attention given to a hybrid structure consisting of two identical planes connected at a single point. Understanding such dynamics is fundamental for applications ranging from spectroscopy to the design of nanostructured materials and devices, where the geometry of the connection between different domains determines the electrical properties and quantum behavior of the system. From a physical standpoint, the study of models involving quantum hybrid

[1] The term "atomtronics" is derived from "atoms" and "electronics," emphasizing its analogy to traditional electronics, where atoms replace electrons as the carriers of information or current.

systems emerged in the context of spectroscopy, where the aim was to understand conduction characteristics in regions with singular geometries, such as halfline-plane junctions. Quantum hybrid systems are now recognized as the most natural mathematical model to describe devices combining one-dimensional and two-dimensional materials, where quantum effects become significant at the nanoscale.

A growing body of research suggests that quantum phenomena, such as quantum coherence, might play a key role in these biological processes, offering an efficient mechanism for energy transfer and information processing. Specifically, studies on photosynthesis have shown evidence of quantum coherence enhancing the efficiency of excitation energy transfer, sparking a broader interest in quantum biology. The challenge in understanding these processes lies in the fact that biological systems operate in an open environment, making it difficult to preserve the delicate quantum features necessary for such phenomena. Unlike isolated systems, open quantum systems are constantly in contact with their surroundings, introducing noise that can disrupt quantum coherence. This raises a fundamental question: How does nature maintain quantum features in open systems? To explore this question, in Part II of the thesis, we focuse on excitation energy transfer in photosynthetic complexes, a biological phenomenon that has recently drawn attention for its potential use in quantum technologies. While classical physics provides a suitable description for many phenomena, it fails to explain the efficiency of certain biological processes, such as those occurring in photosynthetic systems. Excitation energy transfer in photosynthetic organisms occurs through a complex network of chlorophyll molecules, and recent studies suggest that quantum coherence might play a crucial role in optimizing this process. In Part II, we introduce a hybrid quantum-classical approach to model energy transfer in a spin system representing a chain of chlorophyll molecules, interacting with a classical vibrational environment. The theoretical analysis begins with the spin-boson model to understand how the deterministic vibrational motion of the molecular structure affects quantum-coherent excitation transfer. The interaction between the system and an external environment, consisting of a vibrational bath that introduces thermal motion into the model, is treated in a hybrid fashion, considering the environment as a stochastic classical field. The central issue in this research lies in understanding how an open quantum system can maintain its quantum features despite interacting with a noisy environment. To this end, we discuss two main approaches: the fully quantum approach, based on modeling the entire system, and the hybrid quantum-classical approach, which uses a classical description for the environment. The research focuses on exploring the implications of these models in the context of biological processes, particularly in photosynthesis, to determine whether and how quantum features can enhance biological processes.

Throughout the thesis, we will delve into the mathematical and physical implications of both the problems. Part I is dedicated to the description of the mathematical techniques used to study quantum dynamics in hybrid systems, with a focus on nonlinear differential equations and the challenges associated with defining self-adjoint operators in complex geometries. In Part II, we will explore the model for energy transfer in photosynthetic systems, analyzing the implications of quantum coherence in biological processes and proposing new approaches for the mathematical description of the interactions be-

tween the system and the environment. In both cases, our goal is to develop a deeper understanding of the dynamics of complex systems, using advanced mathematical tools to describe and predict quantum behaviors in the presence of nontrivial geometries and external environments.

NLS on quantum Hybrids

Let us first take a step back and focus on quantum hybrids. Quantum hybrids are multidimensional structures on which a quantum dynamics is set: more specifically, different manifolds characterized by different dimensionality are glued together in such a way that a non-trivial dynamics on the whole structure can be defined. The significance of this process of hybridization lies in the specific mathematical technique used to construct such structures that allows us to deal with operators typical of quantum mechanics. In the paper presented in the Chapter 3, we continue the investigation of stationary solutions of nonlinear Schrödinger equations on quantum hybrids started in [4, 5], where a plane + halfline hybrid and a plane + line hybrid were considered (see Figure 1). Here we consider a double plane hybrid, namely a hybrid structure where two identical planes are connected at a single point (see Figure 2). The dynamics is described by a nonlinear Schrödinger equation of the form

$$i\frac{\partial}{\partial t}\Psi = H\Psi + g(\Psi), \qquad \Psi = (z,w) : L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2) \to \mathbb{C}^2$$

where $g : \mathbb{C}^2 \to \mathbb{C}^2$ is a nonlinear function given by

$$g(z,w) = (-|z|^{p_1-2}z, -|w|^{p_2-2}w), \qquad p_1, p_2 > 2$$

and H is a self-adjoint operator on the quantum hybrid (see Section 3.1 for more details). Such a dynamics coincides with the standard NLS dynamics on each plane far from the points where the planes are glued together and allow a connection between the two planes through proper matching conditions that make the operator H a self-adjoint operator.

From the physical point of view, the study of various models involving quantum hybrids began in the context of spectroscopy in order to understand the characteristics of the conduction in regions where the geometry presents a singularity of halfline-plane type (see [41] and Figure 1).

The mathematical interest in this type of models dates back to the late eighties with the papers [33, 34, 36], where the authors considered both hybrids made of a plane and a halfline and hybrids made of two planes connected at a point. The geometry of point contacts is crucial in point-contact spectroscopy since it directly influences the mechanisms of electron transport. When the dimensions of the metallic contact are comparable to or smaller than the electron mean free path, the electron transport becomes ballistic rather than diffusive. In this regime, electrons can traverse the contact without scattering, allowing for a direct study of electron-phonon interactions [41].

Although initially developed for its applications in the latest advancements of solid-state physics, the technique of point-contact spectroscopy has proven to be useful for the characterization of superconducting materials, and in particular for mapping bosonic

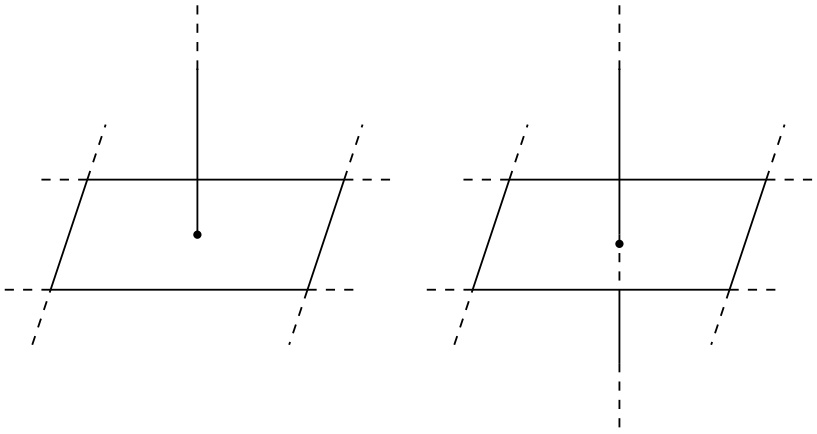


Figure 1: Plane + halfline hybrid (on the left) and plane + line hybrid (on the right).

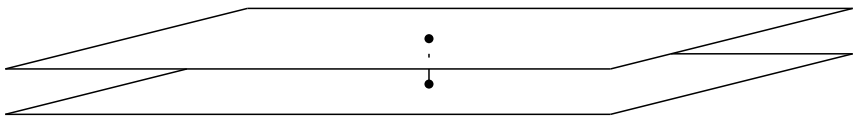


Figure 2: Double-plane hybrid.

and superconducting order parameter spectra through quasiparticle classical and Andreev scattering, respectively [45].

Hybrid quantum systems represent the most natural mathematical modeling even for configurations resulting from the construction of devices based on one-dimensional and two-dimensional materials or nanostructures. [38]. The electrical properties of nano contacts affect the controllability, reliability, and efficiency of the device. Managing current transport in nano contacts is essential for achieving technological advancements [14]. This effectively gives rise to structures that are geometrically similar to hybrids, whose dimensions make quantum effects non-negligible.

From a mathematical point of view, the study of linear and nonlinear PDEs on hybrids represents the generalization and the natural continuation of the well established line of research about linear and nonlinear dynamics on metric graphs. The literature in this field is huge and we provide only some recent results about this topic, especially in the nonlinear setting [1, 6, 8, 9, 10, 17, 18, 20, 21, 28, 30, 31, 43, 46].

Let us mention that an interesting extension can be done also considering $\mathcal{PT}$-symmetric hamiltonians on quantum hybrids [11].

The common and peculiar aspect of the research programs on hybrids and metric graphs lie in the fact that, besides being inspired by physical models, they serve as useful laboratories for the development and application of mathematical techniques. The main difference

between metric graphs and hybrids is that in the latter case the definition of self-adjoint operators is more difficult due to the singular character of the fundamental solution of the Laplacian in dimension higher than one, making the nonlinear problem even more challenging. Even though the present paper discusses a specific example of quantum hybrid as done in [4, 5], the long-term goal is to isolate topological and dimensional properties that distinguish different quantum hybrids from the point of view of the existence and stability of stationary solutions.

Excitation energy transfer in photosynthetic complexes

In the second part, we present a second paper dealing with the theoretical setting for understanding excitation energy transfer in photosynthetic complexes, with a focus on the hybrid quantum-classical approach. Classical physics seems to be not satisfactory to explain some life processes in living systems which are very performant. To give only some examples, it is for the moment not at all understood how our brain, constituted of a dense network of neurons, is able to deal with such an incredibly large amount of information and what is more, even on very short time scales. Vision and olfaction are other examples of biological processes for which traditional (classical) approaches give no satisfactory answer for explaining their efficient functioning. There are indeed several processes in biological organisms for which it is thought that quantum coherence is used by nature in order to enhance the efficiency of the underlying evolution, see for example [67, 69, 71]. However quantum mechanics requires an isolated framework, and in contrast to classical systems, it is very difficult to protect a quantum system from external noise [54, 68, 74]. Furthermore, quantum features are very sensitive to perturbations, fact which makes the implementation of quantum technology so complicated. Thus the essential question which arises spontaneously is: *How does nature maintain quantum features in an open quantum system, which is in permanent contact with a noisy environment*? In this sense, the aim of the second paper is to go a step further in the understanding of the performances of a fundamental biological process, namely the excitation energy transfer in photosynthesis complexes. Some evidence of quantum coherence in the photosynthesis process can be found in [62, 70, 75, 76]. This paper is the follow-up of a first work by one of the authors [73] and it is modelled by the Schrödinger equation (spin-boson model), describing the propagation of an absorbed photon along a spin-chain (representing the chlorophyll molecule-chain) embedded in a vibrational environment. The focus is on the influence of the classical vibrational motion (thermal motion) of the molecular structure (chlorophyll) on the quantum coherent excitation transfer.

The dynamics of open quantum systems has captivated the attention of several researchers in the last years, due to essential applications in quantum computing [55], quantum thermodynamics [72] and quantum biology [48]. The center of activity is the understanding of the effect of the surrounding environment on the central, open quantum system, and the design of simple mathematical models permitting to describe solely the dynamics of interest, namely the one of the central quantum system. Two approaches are mainly considered:

(a) the **fully quantum approach**, which is the most general and precise description,

based on the whole "system + environment" modelling. In order to render the system more tractable, in particular to describe only the central system dynamics, one makes use of the reduced density matrix formalism, taking the partial trace of the full density matrix over the environment, eliminating thus the environmental degrees of freedom and leading to the so-called Master-equation of the central quantum system. This type of asymptotic reduction is mathematically very rigorous.

(b) the **hybrid, quantum-classical approach**, which is an approximate theory, based on a classical description of the (macroscopic) environment. The evolution of the central system is described by a Schrödinger equation, where the Hamiltonian is time-dependent and, depends on external parameters or stochastic fields, which describe the interaction with the environment. The statistical properties of the stochastic fields determine the properties of the environment and have to be carefully chosen. This type of approach is empirical.

Due to the complex structure of realistic environments and of the environment-system interactions, it is rather hard to obtain a Master equation in a rigorous mathematical form (approach (a)). Most of the time, the description of open quantum systems relies on approximations (approach (b)), which are often mathematically not-justified and may lead to erroneous conclusions. The two approaches presented above differ in the way the environment is modelled, namely as a quantum or a classical bath. At high temperatures, the picture of a classical environment (stochastic noise) is a valid description of the environment. However at low temperatures, the vibrational bath cannot be described any more by an external random, classical field, and requires a quantum-mechanical description, taking into account for the back-action of the central system on the environment. For more details about these approaches and their limitations, see [61, 64] and references therein.

Open questions which are for the moment at the heart of the modelling of open quantum systems are: how to model open quantum systems in a precise and also mathematical tractable manner and how to identify clear signatures of quantum phenomena. Is it possible to consider the hybrid approach (b) or is the fully quantum approach (a) necessary. Is it finally possible to show that quantum systems have clear advantages over their classical counterparts *etc.* The goal of such studies is among others to identify clearly if quantum features are actually responsible for an enhancement of biological processes. Chapter 4 tries to give some answers in this direction.

The toy model of this paper is the excitation energy transfer in photosynthesis complexes. The aim is to model mathematically and study numerically how (or if) the interaction with a vibrational environment (heat bath) permits to enhance the transfer of a photon from one end to the other end of a spin-chain, which represents the chlorophyll molecules in a plant leaf. The former paper [73] was based on a fully quantum mechanical approach, and was kept simple in order to be able to do some numerics (only one common environmental bath). However, the model was finally too simple to clearly separate quantum and classical features in the excitation energy transfer. The present

paper focus rather on a hybrid quantum-classical approach. The particular question is to understand the role of the deterministic vibrations of the underlying molecular structure on the quantum-coherent propagation of the excitation through the spin-chain. This is in contrast to a stochastic disturbance by the environment.

The organization of the thesis

In Chapter 1, we recall the definition and the main known results of point interactions. Specifically, we discuss the theory of self-adjoint extensions of symmetric operators through Krein's theory, with a particular interest in the application of this theory to singular objects like quantum graphs or hybrid structures.

Chapter 2 presents some relevant properties of the nonlinear Schrödinger equation (NLS). In particular, we start considering the problem on the euclidean space $\mathbb{R}^n$, reporting results about the well-posedness, conservation laws and particular stationary solutions called standing waves. Then, in Section 2.1 we recall recent results about stationary solutions for nonlinear Schrödinger equations on two specific hybrids, namely the halfline–plane and line–plane hybrids.

Chapter 3 is organized as follows. In Section 3.1 we present the problem of the existence of ground states on the double plane hybrid. In section 3.2, we present the main results about the existence and the properties of ground states. In Section 3.3 we recall some preliminary results, in particular concerning the domain of the energy with point interaction in Subsection 3.3.1, the problem at infinity on the hybrid in Subsection 3.3.2 and Gagliardo-Nirenberg inequalities in Subsection 3.3.3. In Section 3.4 we provide the proof of Theorem 3.2.1 about the existence of ground states. Section 3.5 contains the proof of Theorem 3.2.2 about the properties of ground states, while in Section 3.6 we present the proofs of Theorem 3.2.4 and Theorem 3.2.5, concerning the distribution of mass and the comparison between the strength of the logarithmic singularities on the two planes.

Chapter 4 is organized as follows. In Section 4.2 we present the fundamental Spin-Boson model for the description of the excitation transfer in a spin-chain as well as the driven excitation transfer model, where the transfer is guided by the vibrations of the underlying molecular structure. In Section 4.3 deals with the analytic computations in the case of a chain consisting of $N = 2$ molecules, permitting to understand the cooperation between the deterministic vibrational motion and the quantum excitation transfer. The chapter ends with some conclusions and perspectives.

In Chapter 5 we present some future perspectives, concerning the possibility to use Physics-Informed Neural Networks (PINNs) to solve partial differential equations (PDEs) in complex systems. We recall how the PINNs are able to approximate solutions of PDEs by minimizing a loss function that combines data and physical constraints. Finally, we show how PINNs can be used to solve a nonlinear Schrödinger equation on a particular metric graph, called star graph.

Part I

Chapter 1

Point interactions

1.1 A brief introduction

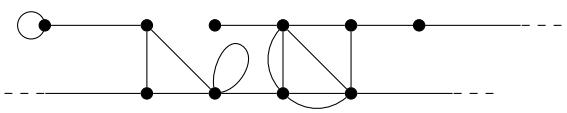
The nonlinear Schrödinger equation (NLS) represent an effective model for the description of the evolution of Bose-Einstein condensates (BECs), reducing the description of the dynamics of many particles to the nonlinear dynamics of one particle only. In particular, the cubic NLS equation reads as

$$\imath\frac{\partial\psi}{\partial t} = -\Delta\psi - |\psi|^2\psi, \qquad \text{on} \quad \mathbb{R}^+ \times \mathbb{R}^n.$$

The mathematical properties of this equation have been extensively studied in the last decades: for a comprehensive treatment of such equation, we refer to [26, 56, 77].
From a mathematical perspective, our aim is to generalize the study of equations of this type in cases where the equation is defined on a multi-dimensional set Ω obtained by gluing together manifolds of different dimensions. In general, we are therefore interested in an equation of this type:

$$\imath\frac{\partial\psi}{\partial t} = -\Delta_\Omega\psi - |\psi|^2\psi, \qquad \text{on} \quad \mathbb{R}^+ \times \Omega,$$

where $-\Delta_\Omega$ is a suitable self-adjoint realization of $-\Delta$ on Ω. The case in which the Laplacian acts on a set Ω composed of sets of dimension one has been analyzed in great detail in recent years and corresponds to the study of quantum graphs (see [19] for an introduction on the topic). A quantum graph is obtained gluing together one-dimensional objects, called edges, at specific points, called vertices. The dynamics inside the edges is governed by the free Laplacian together with a nonlinear term, while the dynamics at the vertices is ruled by specific boundary conditions. The resulting dynamics is not simply obtained by the superposition of the dynamics on the single edges, but it is modified by the presence of such boundary conditions. In an analogous way, the dynamics on hybrids will



be described by the free dynamics inside the single objects composing the whole hybrid, together with specific boundary conditions at the points where these objects are glued together. The operators acting on the hybrid as a whole must be self-adjoint in a suitable Hilbert space. To this end, we will illustrate the main techniques for obtaining interactions supported on points, which will serve as the key components in constructing hybrids.

1.2 Definition of point interactions

In the general framework of quantum mechanics, the focus on *point interactions* is justified by the fact that they represent a completely solvable model. This means that we have explicit analytical expressions for the spectral properties and an explicit representation for the resolvent and the propagator. Point interactions formally correspond to interaction potentials supported on a discrete (finite or infinite) set of points [50] or on a continuous subset [49]. Therefore, the model is particularly effective in describing the behavior of low-energy quantum particles in short-range interaction potentials.

In quantum mechanics, the dynamics of a physical system can be described by the Hamiltonian of the free particle H_0 interacting with a potential V, so that the whole Hamiltonian operator H can be written as $H_0 + V$. The evolution of a quantum system is determined by a one-parameter family of unitary operators $U(t)$, that act on the Hilbert space [23].

Below we will present the construction of point interaction Hamiltonians using the theory of self-adjoint extensions of symmetric operators. If one wants to describe formally a Hamiltonian like $H = H_0 + V$, with V concentrated at some points only, the first idea is to write H as

$$H = -\Delta + \sum_{y \in Y} \lambda_y \delta_y(\cdot) \tag{1.1}$$

where Δ denotes the self-adjoint Laplacian in $L^2(\mathbb{R}^n)$ with domain $H^2(\mathbb{R}^n)$. Here $n = 1, 2, 3$ is the dimension of the underlying configuration space, Y denotes the set of geometric parameters of the interaction, λ_y the dynamic ones, and δ_y is the Dirac $\delta-$function at y (i.e., the unit measure concentrated at y). The quantum mechanical particle therefore moves under the influence of a 'contact potential' generated by 'point sources' that are situated in y and of strengths λ_y.

In this chapter, we will focus on the dynamics of N particles in dimension n subject to a set of point interactions in Y. From a physical point of view, point interactions are introduced to model situations in which a particle is subjected to a very intense force on a short interaction distance with respect to the particle's typical wavelength.

1.3 Construction of point interaction Hamiltonians via Krein theory

Expression (1.1) is only formal since it does not define a self-adjoint operator in $L^2(\mathbb{R}^n)$. There are many different ways to give a rigorous characterization of the formal expression

(1.1), but we will focus on a particular method that makes use of the Krein's theory.

The basic idea is that δ-type potentials at the points y_i, with $i = 1, \dots, N$, can only affect functions that are non-zero at these points. Therefore, a Hamiltonian with point interactions must reduce to the free Hamiltonian when applied to regular functions that are zero at these points. Hence, the operator must satisfy

$$Hu = -\Delta u, \quad \forall u \,:\, \exists B_{\varepsilon_i}(y_i) : u(x) = 0 \;\; \forall x \in B_{\varepsilon_i}(y_i),\, i = 1, \dots, N.$$

where $B_{\epsilon_i}(y_i)$ is a small ball of radius ε_i centered at y_i. In fact, particles described by wave functions of this type, which are zero around the points where the interactions take place, do not feel the presence of the potential, and behave as free particles.

Any possible mathematical definition of a self-adjoint operator H in $L^2(\mathbb{R}^n)$ of the form (1.1) should take into account the fact that, on the space $C_0^\infty(\mathbb{R}^n \setminus \{y_1, \dots, y_N\})$, H should coincide with $-\Delta$. Hence, it is reasonable to consider the following restriction of the Laplace operator:

$$\widehat{H} = -\Delta, \qquad \mathcal{D}(\widehat{H}) = C_0^\infty(\mathbb{R}^n \setminus \{y_1, \dots, y_N\}).$$

Let us observe two relevant things in the construction of the self-adjoint extension. The first one is that if we consider any $f \in L^2(\mathbb{R}^n)$, we have that

$$f \in \mathcal{D}(\widehat{H}^*) \iff F(g) = \langle f, \widehat{H} g \rangle \;\text{ is bounded }\; \forall g \in \mathcal{D}(\widehat{H}).$$

The function g is zero around the points y_i, whereas the function f can takes arbitrary values around that point, and it can even diverge as long as they stay in $L^2(\mathbb{R}^n)$. Hence, the domain of $\widehat{H}^*$ is larger than the domain of $\widehat{H}$. We can conclude that $\widehat{H}$ is symmetric but not self-adjoint in $L^2(\mathbb{R}^n)$.
The second relevant thing is that $\widehat{H}$ has at least one self-adjoint extension, i.e. $H_0 = -\Delta$ with $D(H_0) = H^2(\mathbb{R}^n)$, which corresponds to the Hamiltonian of the free particle, where

$$H^2(\mathbb{R}^n) = \left\{ f : \mathbb{R}^n \to \mathbb{R} \,|\, \|f\|_{H^2}^2 = \int_{\mathbb{R}^2} (1 + |k|^2)^2 \left| \widehat{f}(k) \right|^2 dk < +\infty \right\}.$$

At this point we can give the following definition:

Definition 1.3.1. The Laplace operator with point interaction in $\{y_1, \dots y_N\}$, is defined as any non-trivial self-adjoint extension of $\widehat{H}$, i.e. any self-adjoint extension of $\widehat{H}$ that does not coincide with H_0.

Our goal is to determine all the nontrivial self-adjoint extensions. Let us first focus on the domain of the adjoint $\widehat{H}^*$. Since

$$\langle \psi, -\Delta \phi \rangle = \langle -\Delta \psi, \phi \rangle, \qquad \forall \psi \in H^2(\mathbb{R}^n) \;\text{ and }\; \forall \phi \in \mathcal{D}(\widehat{H}),$$

and, by the Schwartz's inequality, it holds that

$$|(-\Delta \psi, \phi)| \leq \|\psi\|_{H^2} \|\phi\|_{L^2}, \;\; \forall \psi \in H^2(\mathbb{R}^n),$$

then the functional $F(\phi) = \langle \psi, -\Delta\phi \rangle$, defined in $\mathcal{D}(\widehat{H})$, is bounded $\forall \psi \in H^2(\mathbb{R}^n)$, hence $H^2(\mathbb{R}^n) \subseteq \mathcal{D}(\widehat{H}^*)$.

Let us define the Green's functions for the Laplacian as the solutions of the distributional equation $(-\Delta - z)\mathcal{G}_i^z = \delta_{y_i}$, with $z \in \mathbb{C} \setminus \mathbb{R}^+$. Since $\mathcal{G}_i^z \in L^2(\mathbb{R}^n)$, it can be shown that

$$\langle \mathcal{G}_i^z, \widehat{H}\phi \rangle = \langle \widehat{H}^* \mathcal{G}_i^z, \phi \rangle = \langle -\Delta \mathcal{G}_i^z, \phi \rangle = \langle z\mathcal{G}_i^z, \phi \rangle, \qquad \forall \phi \in \mathcal{D}(\widehat{H}) \text{ with } i = 1, \dots, N$$

hence $\mathcal{G}_i^z$ is an eigenfunction of $\widehat{H}^*$ with respect to the eigenvalue z. The only other solutions are given by the derivatives of $\mathcal{G}_i^z$. Denote with N_z the space generated by $\mathcal{G}_i^z$ and by its derivatives, if such derivatives belong to $L^2(\mathbb{R}^n)$: it is straightforward that $N_z \subset L^2(\mathbb{R}^n)$.
We can distinguish the following cases, taking into account the dimension n:

i) $n = 1$. $\mathcal{G}_i^z, (\mathcal{G}_i^z)' \in L^2(\mathbb{R})$, $i = 1, \dots, N$, with $\dim(N_z) = 2N$;

ii) $n = 2, 3$. $\mathcal{G}_i^z \in L^2(\mathbb{R}^n)$, $i = 1, \dots, N$, with $\dim(N_z) = N$;

iii) $n > 3$. $\mathcal{G}_i^z \notin L^2(\mathbb{R}^n)$, $i = 1, \dots, N$, and $\dim(N_z) = 0$.

Let us observe that $H^2(\mathbb{R}^n), N_z \subset \mathcal{D}(\widehat{H}^*)$, with $z \in \mathbb{C} \setminus \mathbb{R}^+$, and that

$$H^2(\mathbb{R}^n) \cup N_z = \mathcal{D}(\widehat{H}^*).$$

The functions in the domain $\mathcal{D}(\widehat{H}^*)$ can be expressed as a linear combination of functions in $L^2(\mathbb{R}^n)$ and in N_z, with fixed $z \in \mathbb{C} \setminus \mathbb{R}^+$.
There is also an alternative description of the functions belonging to the domain $\mathcal{D}(\widehat{H}^*)$. To introduce this representation, let us consider $z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}^+$ with $z_1 \neq z_2$, and define $\Phi_i = \mathcal{G}_i^{z_1} - \mathcal{G}_i^{z_2}$, so that

$$\begin{aligned} &(-\Delta - z_1)\mathcal{G}_i^{z_1} - (-\Delta - z_2)\mathcal{G}_i^{z_2} = 0 \\ &\Delta\Phi_i = \Delta(\mathcal{G}_i^{z_1} - \mathcal{G}_i^{z_1}) = -z_1\mathcal{G}_i^{z_1} + z_2\mathcal{G}_i^{z_2} \in L^2(\mathbb{R}^n), \end{aligned}$$

thus $\Phi_i = \mathcal{G}_i^{z_1} - \mathcal{G}_i^{z_2} \in H^2(\mathbb{R}^n)$. Therefore, functions in $\mathcal{D}(\widehat{H}^*)$ can be written as a linear combination of functions $f \in H^2(\mathbb{R}^n)$ such that $f(y_i) = 0$ for $i = 1, \dots, N$ and functions belonging to N_{z_1} and N_{z_2}, with $z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}^+$ and $z_1 \neq z_2$.
This is a special case of Von Neumann's formula having more general validity:

Given a densely defined and symmetric operator A on a Hilbert space $\mathcal{H}$, then any function $f \in \mathcal{D}(A^*)$ can be uniquely decomposed in this way:

$$f = f_0 + f_z + f_{\overline{z}}$$

with $f_0 \in \mathcal{D}(\overline{A})$, $f_z, f_{\overline{z}}$ are eigenfunction of A^* respect to z and $\overline{z}$, and:

$$A^* f = \overline{A} f_0 + z f_z + \overline{z} f_{\overline{z}}. \tag{1.2}$$

Formula (1.2) gives us a method for constructing self-adjoint extensions of $\widehat{H}$. We consider the action of the adjoint $\widehat{H}^*$ on the spaces N_z and $N_{\overline{z}}$ and identify proper subspaces on which $\widehat{H}^*$ acts as a self-adjoint operator. Different choices of subspaces will correspond to different self-adjoint extensions of $\widehat{H}$. If $n > 3$, the N_z spaces are empty, thus it is not possible to construct any non trivial self-adjoint extension of $\widehat{H}$.

1.4 Construction of point interactions in dimension three

In this section, we focus on the construction of self-adjoint operators in dimension three. More specifically, we study the case of a point interaction with a single centre y: indeed, the description of a simple case give more relevance to the method itself.
Let us introduce the Green's function of the Laplace operator in dimension three centered at the point y, that is the function

$$\mathcal{G}^z(x) = \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|}$$

Applying the Von Neumann decomposition formula introduced before, we can write the domain of $\widehat{H}^*$ as

$$\mathcal{D}(\widehat{H}^*) = \{f \in L^2(\mathbb{R}^3) : f = f_0 + \beta\mathcal{G}^z(\cdot - y) + \gamma\mathcal{G}^{\overline{z}}(\cdot - y), f_0 \in H^2(\mathbb{R}^3) : f_0(y) = 0\},$$

while the action of $\widehat{H}^*$ is given by

$$\widehat{H}^* f = \widehat{H}^*(f_0 + \beta\mathcal{G}^z(\cdot - y) + \gamma\mathcal{G}^{\overline{z}}(\cdot - y)) = -\Delta f_0 + \beta z\mathcal{G}^z(\cdot - y) + \gamma\overline{z}\mathcal{G}^{\overline{z}}(\cdot - y).$$

We now look for subspaces of N_z and $N_{\overline{z}}$ in which $\widehat{H}^*$ acts as a symmetric operator. To do this, we observe that the expression

$$(\beta\mathcal{G}^z(\cdot - y) + \gamma\mathcal{G}^{\overline{z}}(\cdot - y), \widehat{H}^*(\beta\mathcal{G}^z(\cdot - y) + \gamma\mathcal{G}^{\overline{z}}(\cdot - y))) = (|\beta|^2 z + |\gamma|^2\overline{z})\|\mathcal{G}^z\|^2 + 2\mathrm{Re}(\overline{\gamma}\beta(\mathcal{G}^{\overline{z}}, \mathcal{G}^z)),$$

and turns out to be real valued if and only if

$$|\beta| = |\gamma| \iff \gamma = e^{i\phi}\beta \quad \text{for some } \phi \in \mathbb{R}.$$

Therefore, there exists a one-parameter family of self-adjoint extensions of $\widehat{H}$, which depends on ϕ and y but we will call again $\widehat{H}$, such that the domain is given by

$$\mathcal{D}(\widehat{H}) = \{f \in L^2(\mathbb{R}^3) : f = f_0 + \beta\mathcal{G}^z(\cdot - y) + \beta e^{i\phi}\mathcal{G}^{\overline{z}}(\cdot - y)\}$$

and the action reads as

$$\widehat{H} f = -\Delta f_0 + \beta\, z\, \mathcal{G}^z(\cdot - y) + \beta\, e^{i\phi}\, \overline{z}\, \mathcal{G}^{\overline{z}}(\cdot - y).$$

By writing $\mathcal{G}_\lambda = \mathcal{G}^{z=-\lambda}$, $\lambda > 0$, we can verify that

$$\mathcal{G}^z(x-y) + e^{i\phi}\mathcal{G}^{\overline{z}}(x-y) = (1+e^{i\phi})\mathcal{G}_\lambda(x-y) + (1+e^{i\phi})\left(\alpha + \frac{\sqrt{\lambda}}{4\pi}\right) + g_0,$$

where g_0 vanishes for $x = y$ and α satisfies the formula

$$\alpha = \frac{\mathrm{Re}\sqrt{z}}{4\pi}\tan\left(\frac{\phi}{2}\right) - \frac{\mathrm{Im}(\sqrt{z})}{4\pi}.$$

Putting all together, we get that

$$\begin{aligned} f(x) &= f_0(x) + \beta[\mathcal{G}^z(x-y) + e^{i\phi}\mathcal{G}^{\overline{z}}(x-y)] \\ &= \underbrace{f_0(x) + \beta[(1+e^{i\phi})\left(\alpha + \frac{\sqrt{\lambda}}{4\pi}\right) + g_0(x)]}_{\Phi_\lambda(x)} + \underbrace{\beta(1+e^{i\phi})}_{q}\mathcal{G}_\lambda(x-y) \\ &= \Phi_\lambda(x) + q\mathcal{G}_\lambda(x-y), \end{aligned}$$

thus for every $\alpha \in \mathbb{R}$ we obtain a self-adjoint extension with domain and action given respectively by

$$\mathcal{D}(\widehat{H}) = \left\{ f \in L^2(\mathbb{R}^3) : f = \Phi_\lambda + q\,\mathcal{G}_\lambda(\cdot - y),\ \Phi_\lambda \in H^2(\mathbb{R}^3),\ q = \frac{\Phi_\lambda(y)}{\alpha + \frac{\sqrt{\lambda}}{4\pi}} \right\} \tag{1.3}$$

and

$$\widehat{H}f = \widehat{H}(\Phi_\lambda + q\,\mathcal{G}_\lambda(\cdot - y)) = -\Delta\Phi_\lambda - q\lambda\mathcal{G}_\lambda(\cdot - y).$$

Remark 1.4.1. Any element of the domain can be written as the sum of a regular term $\Phi_\lambda \in H^2(\mathbb{R}^3)$ and a singular term $q\mathcal{G}_\lambda \in L^2(\mathbb{R}^3)$. In addition, the relation between q and $\Phi_\lambda(y)$ in (1.3) represents the boundary condition that a function f of the domain has to satisfy at the point y.

In order to deduce information about the spectrum, we have to analyze the resolvent operator $(\widehat{H} + z)^{-1}$, for z real and positive. Let us first recall that the action of $\widehat{H}$ on $\mathcal{D}(\widehat{H})$ can be expressed also as

$$(\widehat{H} + \lambda)f = (-\Delta + \lambda)\Phi_\lambda. \tag{1.4}$$

Therefore, by using (1.4), for every function $g(x) \in L^2(\mathbb{R}^3)$ it follows that

$$(\widehat{H} + \lambda)^{-1}g = \Phi_\lambda + q\mathcal{G}_\lambda(\cdot - y). \tag{1.5}$$

If we apply $(\widehat{H} + \lambda)$ on both members of the last equation, then we get that

$$g = (\widehat{H} + \lambda)\Phi_\lambda + q(\widehat{H} + \lambda)\mathcal{G}_\lambda(\cdot - y) = (-\Delta + \lambda)\Phi_\lambda,$$

so that that $\Phi_\lambda = \mathcal{G}_\lambda g$. By substituting this expression in (1.5), there results that

$$(\widehat{H} + \lambda)^{-1}g = \mathcal{G}_\lambda g + \frac{1}{\alpha + \sqrt{\lambda}/4\pi}\mathcal{G}_\lambda(\cdot - y)\,(\mathcal{G}_\lambda g)\,(y)$$

Given this expression of the resolvent, we are able to deduce the spectral properties of $\widehat{H}$. In particular, the spectrum of $\widehat{H}$ is given by

$$\sigma(\widehat{H}) = [0, \infty) \quad \alpha \geqslant 0$$
$$\sigma(\widehat{H}) = \left\{-16\pi^2\alpha^2\right\} \cup [0, \infty) \quad \alpha < 0$$

where the continuous part $[0, \infty)$ is purely absolutely continuous.
For $\alpha < 0$ there is a unique simple eigenvalue corresponding to the normalised eigenfunction

$$\psi_\alpha(x) = \sqrt{-2\alpha}\frac{e^{(4\pi\alpha|x-y|)}}{|x-y|}$$

For every $\alpha \in \mathbb{R}$ and for every positive value of the energy, it corresponds a generalized eigenfunction given by

$$\psi_\alpha(k, x) = \frac{1}{(2\pi)^{3/2}}\left(e^{ik\cdot x} - \frac{e^{ik\cdot y}}{\alpha - i|k|/(4\pi)}\frac{e^{(i|k||x-y|)}}{|x-y|}\right)$$

where $|k|^2 = E$.

Notice that the free Laplacian is obtained formally in the limit $\alpha \to \infty$, showing that one cannot consider α as the significative dynamical parameter. Its physical meaning becomes clear studying scattering theory for point interaction Hamiltonians. In this context, it can be proved that α is the inverse of the scattering length associated to the operator $\widehat{H}$. The explicit form of the spectral decomposition of $\widehat{H}$, in terms of the eigenfunctions (in the case $\alpha < 0$) and of the generalized eigenfunctions, allows us to have an almost explicit formula for the solutions of the Schrödinger equation

$$i\frac{\partial\psi_t}{\partial t} = \widehat{H}\,\psi_t.$$

$\psi_0 \in \mathcal{D}(\widehat{H})$. More specifically, given an initial datum $\psi_0 \in \mathcal{D}(\widehat{H})$, then the solution ψ_t at time t is given by the free-propagation of the initial datum plus a term that represents the effect of spherical waves generated at the interaction centre, i.e.

$$\psi_t(x) = \left(U(t)\psi_0\right)(x) + i\int_0^t dsU(t-s, |x-y|)q(s) \tag{1.8}$$

where $U(t)$ is the propagator of the free Schrödinger equation with kernel given by

$$U\left(t; x-x'\right) = e^{i\Delta t}\left(x-x'\right) = \frac{e^{i\frac{|x-x'|^2}{4}}}{(4\pi it)^{3/2}}.$$

Let us finally note that, if (1.8) is the solution of the Schrödinger equation corresponding to an initial condition $\psi_0 \in D(\widehat{H})$, then the function $q(t)$ satisfies the integral equation

$$q(t) + 4\sqrt{i\pi}\alpha\int_0^t ds\frac{q(s)}{\sqrt{t-s}} = 4\sqrt{i\pi}\int_0^t ds\frac{\left(U(s)\psi_0\right)(y)}{\sqrt{t-s}}. \tag{2.21}$$

Formally, the dynamics of the whole wave function can be reduced to the dinamics of the charge $q(t)$ through equation (2.21).

1.5 Construction of point interactions in dimension two

In this section, we will introduce the objects that are useful to define self-adjoint operators with a point interaction in dimension two.
For every $\lambda > 0$, we denote by $\mathcal{G}_\lambda$ the only $L^2(\mathbb{R}^2)$ solution of the distributional equation $(-\Delta + \lambda)\mathcal{G}_\lambda = \delta_0$, where δ_0 is the Dirac-delta distribution centered at $x = 0$.
Such solution can be expressed in terms of a special function as

$$\mathcal{G}_\lambda(x) = \mathcal{G}_1(\sqrt{\lambda}x) = \frac{1}{2\pi} K_0(\sqrt{\lambda}|x|),$$

where K_0 is the Macdonald's function of order zero [83]. In order to easy the notation, we will simply write $\mathcal{G}$ in place of $\mathcal{G}_1$. There are some relevant features of the function $\mathcal{G}_\lambda$:

i) it is positive, radial and strictly decreasing;

ii) it vanishes exponentially fast, as $|\mathbf{x}| \to +\infty$;

iii) $\mathcal{G}(x) = -\frac{\log|x|}{2\pi} + \theta + o(1)$ as $x \to 0$, with $\theta := \frac{\gamma - \log 2}{2\pi}$, where γ denotes the Eulero-Mascheroni constant.

Let us finally remark that for every $\lambda > 0$ it holds that $\mathcal{G}_\lambda \in L^p(\mathbb{R}^2)$ for every $p \in [1, +\infty)$, while $\mathcal{G}_\lambda \notin H^1(\mathbb{R}^2)$. Following the same approach of the previous section, we can define also a point interaction in dimension two. Let us denote with $\widehat{H}$ the self-adjoint operator in $L^2(\mathbb{R}^2)$, given by Laplacian with a delta interaction of "strength" α placed at $x = 0$.
If $n = 2$, then the domain of the operator $\widehat{H}$ is given by

$$\mathcal{D}(\widehat{H}) = \{\psi \in L^2(\mathbb{R}^2) \,|\, \psi = \phi_\lambda + q\,\mathcal{G}_\lambda, \phi_\lambda \in H^2(\mathbb{R}^2)\,,\, q \in \mathbb{C}\,,\, q = \Gamma_\alpha(\lambda)\phi_\lambda(0)\}$$

with

$$\Gamma_\alpha(\lambda) = \frac{2\pi}{2\pi\alpha + \gamma + \log(\sqrt{\lambda}/2)}, \qquad \alpha \in \mathbb{R}.$$

Taking into account the decomposition $\psi = \phi_\lambda + q\mathcal{G}_\lambda$ in the definition of the operator domain, the action of the operator is given by

$$\widehat{H}\psi = -\Delta\phi_\lambda - \lambda q \mathcal{G}_\lambda, \qquad \forall \psi \in \mathcal{D}(\widehat{H}).$$

If $n = 2$, then $\widehat{H}$ has a simple negative eigenvalue e_α for any $\alpha \in \mathbb{R}$ with ϕ_α the corresponding normalized eigenvector given by

$$\phi_\alpha(x) = N_\alpha K_0(2e^{-2(2\pi\alpha+\gamma)}|x|), \qquad \alpha \in \mathbb{R}$$

where N_α is a normalization constant whose explicit value is irrelevant for our analysis.

1.6 Quantum hybrids

In this section, we will focus on the definition of a dynamics governed by Schrödinger equations and set on singular manifolds consisting of two or more simple parts glued together at specific points: the final aim is to define a non-trivial dynamics on such structures,

namely a dynamics that do not create a separation between the different parts of the singular manifold itself. Such structures are called quantum hybrids. The significance of this process of hybridization lies in the specific mathematical technique used to construct such dynamics and allows us to deal with operators typical of quantum mechanics. First, we will present a prototypical case, introduced in [33] and called the halfline-plane hybrid: such structure, denoted in the following by $\mathcal{J}$, consists of a halfline whose origin is connected to a plane (as in Figure 1.1) and on which a nontrivial dynamics is defined. Then, we will present some result involving a different kind of hybrid, made up of two planes connected at point P and denoted in the following by $\mathcal{I}$ (as in Figure 1.2). In this paragraph, we briefly outline the rigorous definition of the class of self-adjoint operators one can define on quantum hybrids such as $\mathcal{J}$ and $\mathcal{I}$. The first result that appeared in the literature is contained in the paper [36].

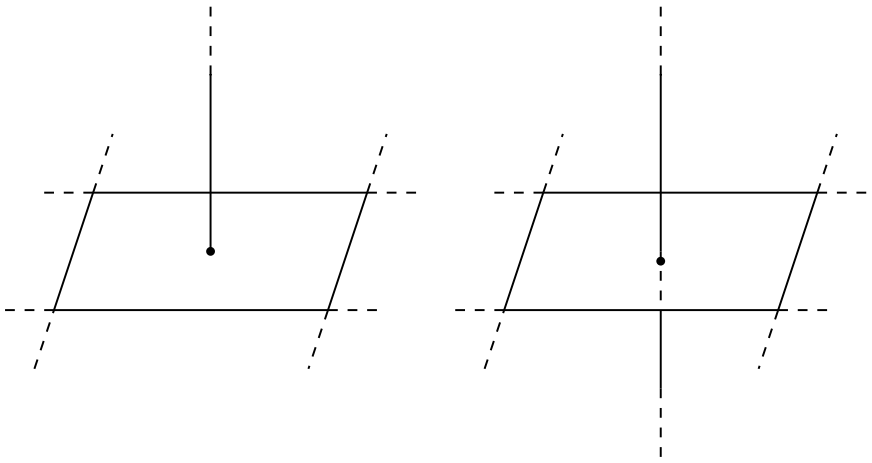


Figure 1.1: Plane + halfline hybrid (on the left) and plane + line hybrid (on the right).

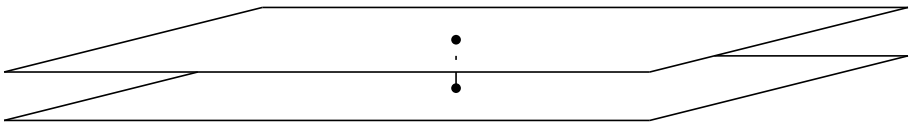


Figure 1.2: Double-plane hybrid.

1.6.1 The plane + halfline hybrid

Given the hybrid $\mathcal{J}$, we can define functions on $\mathcal{J}$ as $U : \mathcal{J} \to \mathbb{C}$, where $U = (u_1, u_2)$, with $u_1 : \mathbb{R}^+ \to \mathbb{C}$ and $u_2 : \mathbb{R}^2 \to \mathbb{C}$. We now rigorously define a class of self-adjoint operators $H_{\mathcal{J}} : \mathcal{D}(H_{\mathcal{J}}) \subset L^2(\mathcal{J}) \to L^2(\mathcal{J})$, obtained as self-adjoint extensions of the symmetric operator $H_{sym} = H_1 \oplus H_2$, where

$$H_1 : C_c^\infty(\mathbb{R}) \subseteq L^2(\mathbb{R}^+) \to L^2(\mathbb{R}^+), \qquad H_1 u = -u''.$$

and

$$H_2 : C_c^\infty(\mathbb{R}^2\backslash\{0\}) \subseteq L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2), \qquad H_2 v = -\Delta v.$$

Before defining $H_{\mathcal{J}}$, it is necessary to define the self-adjoint extensions of H_1 on $L^2(\mathbb{R}^+)$ and of H_2 on $L^2(\mathbb{R}^2)$ respectively. The self-adjoint extensions of H_1 are given (see, e.g., [16, Section 6.2.2]) by the one parameter family of operators H_1^α, with $\alpha \in \mathbb{R} \cup \{\pm\infty\}$, with domain

$$\mathcal{D}(H_1^\alpha) := \{u \in H^2(\mathbb{R}^+) : u'(0) = \alpha u(0)\}$$

and action given by $H_1^\alpha u = -u''$ on $\mathbb{R}^+$, for all $u \in \mathcal{D}(H_1^\alpha)$. The condition $u'(0) = \alpha u(0)$ represents the boundary condition. In particular, we can distinguish three cases; if $\alpha \in \mathbb{R}\backslash\{0\}$, then the condition is a delta (or Robin) boundary condition, if $\alpha = 0$, then we have Neumann boundary condition, if instead $\alpha = \pm\infty$, then the boundary condition reduces to the Dirichlet boundary condition. In particular, if $\alpha > 0$, then the boundary condition is called **repulsive**, while if $\alpha < 0$, then the boundary condition is called **attractive**. The quadratic form $Q_\alpha(u) : H^1(\mathbb{R}^+) \to \mathbb{R}$ associated with H_1^α is defined as follows:

$$Q_\alpha(u) := \|u'\|^2_{L^2(\mathbb{R}^+)} + \alpha|u(0)|^2 \quad \forall\, u \in H^1(\mathbb{R}^+).$$

Finally, from an analysis of the spectral properties of H_1^α, it is known (see, e.g., [16, Section 6.2.2]) that

$$\sigma(H_1^\alpha) = \begin{cases} [0, +\infty), & \text{if } \alpha \geq 0 \\ \{-\alpha^2\} \cup [0, +\infty), & \text{if } \alpha < 0, \end{cases}$$

where $[0, +\infty)$ is the essential spectrum and $-\alpha^2$ is the unique eigenvalue, that can be characterized as

$$-\alpha^2 = \inf_{u \in H^1(\mathbb{R}^+)\backslash\{0\}} \frac{Q_\alpha(u)}{\|u\|^2_{L^2(\mathbb{R}^+)}}.$$

On the other hand, the self-adjoint extensions of H_2 are given (see, e.g., [44, Chapter I.5]) by the one parameter family of operators H_2^σ, with $\sigma \in \mathbb{R} \cup \{\pm\infty\}$, whose domain and action are given by

$$\mathcal{D}(H_2^\sigma) = \left\{ u \in L^2(\mathbb{R}^2) : \exists\, q \in \mathbb{C}\,,\, \lambda > 0 \text{ s.t. } u - q\mathcal{G}_\lambda =: \phi_\lambda \in H^2(\mathbb{R}^2)\,,\, \phi_\lambda(0) = (\sigma + \theta_\lambda)q \right\}$$

and

$$H_2^\sigma\, u = -\Delta\phi_\lambda - q\,\lambda\,\mathcal{G}_\lambda, \qquad \forall\, u = \phi_\lambda + q\mathcal{G}_\lambda \in \mathcal{D}(H_2^\sigma),$$

where $\mathcal{G}_\lambda : \mathbb{R}^2 \setminus \{0\} \to \mathbb{R}^+$ is the Green's function of $-\Delta + \lambda$ and

$$\theta_\lambda := \frac{\log(\sqrt{\lambda}) - \log(2) + \gamma}{2\pi},$$

with γ denoting the Euler-Mascheroni constant.

Note that in the following ϕ_λ and $q\mathcal{G}_\lambda$ are given as the *regular part* and *singular part*, respectively, of an element in $\mathcal{D}(H_2^\sigma)$. In addition, q is usually called *charge*, and it is a important parameter uniquely determined for all $u \in \mathcal{D}(H_2^\sigma)$.

The quadratic form $Q_\sigma(u) : \mathcal{D} \to \mathbb{R}$ associated with H_2^σ is defined by

$$Q_\sigma(u) := \|\nabla\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} + \lambda\Big(\|\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} - \|u\|^2_{L^2(\mathbb{R}^2)}\Big) + |q|^2(\sigma + \theta_\lambda), \qquad \forall u \in \mathcal{D},$$

where

$$\mathcal{D} := \{u \in L^2(\mathbb{R}^2) : \exists\, q \in \mathbb{C} \,:\, u - q\mathcal{G}_\lambda := \phi \in H^1(\mathbb{R}^2)\}.$$

The boundary condition $\phi_\lambda(0) = (\sigma + \theta_\lambda)q$ yields a delta-type boundary condition only if $\phi \in \mathbb{R}$. The spectrum of H_2^σ (see, e.g., [44, Chapter I.5]) is given by

$$\sigma(H_2^\sigma) = \{-4e^{-4\pi\sigma-2\gamma}\} \cup [0, +\infty),$$

where $[0, +\infty)$ is again the essential spectrum and $-4e^{-4\pi\sigma-2\gamma}$ is the unique eigenvalue: as for the eigenvalue on the halfline, it is possible to provide a variational characterization of it, given by

$$-4e^{-4\pi\sigma-2\gamma} = \inf_{u\in\mathcal{D}\setminus\{0\}} \frac{Q_\sigma(u)}{\|u\|^2_{L^2(\mathbb{R}^2)}}.$$

Since the operator H_2^σ has a negative eigenvalue for every value of $\sigma \in \mathbb{R}$, the delta is called *attractive* for every $\sigma \in \mathbb{R}$: this marks an important difference with the one-dimensional case.

Let us consider a system made up of a halfline connected to a plane at the origin. We are now ready to define the self-adjoint extensions of the Laplacian on the hybrid $\mathcal{J}$. To this aim, we follow the classification established by Exner and Sêba in [33, 34]. In particular, we report only the definition of the self-adjoint operators $H_\mathcal{J}$ belonging to a class that the authors call class I. The hybrid $\mathcal{J}$, namely

$$L^2(\mathcal{J}) = L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^2) = \{U = (u_1, u_2) : \mathcal{J} \to \mathbb{C} : u_1 \in L^2(\mathbb{R}^+), u_2 \in L^2(\mathbb{R}^2)\},$$

and the symmetric operator $H_{sym} = H_1 \oplus H_2$. By making use of the Krein's self-adjoint extension theory, it is possible to define for any $\alpha, \sigma \in \mathbb{R}$ and $\beta \geq 0$ the self-adjoint operator $H_\mathcal{J} : \mathcal{D}(H_\mathcal{J}) \subset L^2(\mathcal{J}) \to L^2(\mathcal{J})$, whose domain and action are given respectively by

$$\mathcal{D}(H_\mathcal{J}) := \Bigg\{U = (u_1, u_2) \in L^2(\mathcal{J}) \,:\, u_1 \in H^2(\mathbb{R}^+),\, \exists\, q \in \mathbb{C}, \lambda > 0 \,:\, u_2 - q\,\mathcal{G}_\lambda := \phi_\lambda \in H^2(\mathbb{R}^2),$$
$$\begin{pmatrix} u_1'(0) \\ \phi_\lambda(0) - \theta_\lambda q \end{pmatrix} = \begin{pmatrix} \alpha & -\beta \\ -\beta & \sigma \end{pmatrix} \begin{pmatrix} u_1(0) \\ q \end{pmatrix} \Bigg\} \quad (1.9)$$

and

$$H_{\mathcal{J}}U = (H_1^{\alpha}u_1, H_2^{\sigma}u_2).$$

The boundary condition in (1.9) can be written also as follows

$$\begin{cases} u_1'(0) = \alpha u_1(0) - \beta q \\ \phi_\lambda(0) = -\beta u_1(0) + (\sigma + \theta_\lambda)q. \end{cases}$$

Moreover, the quadratic form $Q_{\mathcal{J}} : \widehat{\Lambda} \to \mathbb{R}$ associated with the operator $H_{\mathcal{J}}$ has domain

$$\widehat{\Lambda} := H^1(\mathbb{R}^+) \times \mathcal{D} = \{U = (u_1, u_2) \in L^2(\mathcal{I}) : u_1 \in H^1(\mathbb{R}^+) \text{ and } u_2 \in \mathcal{D}\},$$

and action

$$\begin{aligned} Q_{\mathcal{J}}(U) &= Q_\alpha(u_1) + Q_\sigma(u_2) - 2\beta \mathrm{Re}\{q\overline{u_1(0)}\} \\ &= \|u_1'\|^2_{L^2(\mathbb{R}^+)} + \alpha|u_1(0)|^2 + \|\nabla\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} + \lambda(\|\phi_\lambda\|_2^2 - \|u_2\|_2^2) \\ &+ |q|^2(\sigma + \theta_\lambda) + 2\mathrm{Re}\{\beta\, q\, \overline{u_1(0)}\} \end{aligned}$$

In particular, the quadratic form $Q_{\mathcal{J}}$ is symmetric and

$$Q_{\mathcal{J}}(U) = \langle U, H_{\mathcal{J}}U\rangle_{L^2(\mathcal{J})}, \qquad \forall U \in \mathcal{D}(H_{\mathcal{J}}).$$

1.6.2 The double Plane hybrid

Let $\mathcal{I}$ be the double-plane hybrid, that is, a system made up of two planes connected to a point P. Let us now consider the Hilbert space of such a system, given by

$$L^2(\mathcal{I}) := L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2) = \{U = (u_1, u_2) : \mathcal{I} \to \mathbb{C} : u_1 \in L^2(\mathbb{R}^2), u_2 \in L^2(\mathbb{R}^2)\},$$

and the symmetric operator $H_p = H_2 \oplus H_2$. Therefore, by Krein's theory of self-adjoint extensions, it is possible to define for every $\sigma_1, \sigma_2 \in \mathbb{R}$ and $\beta \geqslant 0$ the self-adjoint operator $H : \mathcal{D}(H) \subset L^2(\mathcal{I}) \to L^2(\mathcal{I})$, with domain

$$\mathcal{D}(H) := \Bigg\{ U = (u_1, u_2) \in L^2(\mathcal{I}) \,:\, \exists\, q_i \in \mathbb{C}, \lambda_i > 0 \,:\, u_i - q_i\, \mathcal{G}_{\lambda_i} := \phi_{i,\lambda_i} \in H^2(\mathbb{R}^2), \\ \begin{pmatrix} \phi_{1,\lambda_1}(0) - \theta_{\lambda_1} q_1 \\ \phi_{2,\lambda_2}(0) - \theta_{\lambda_2} q_2 \end{pmatrix} = \begin{pmatrix} \sigma_1 & -\beta \\ -\beta & \sigma_2 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \Bigg\} \quad (1.10)$$

and action

$$HU = (-\Delta\phi_{1,\lambda_1} - \lambda_1 q_1 \mathcal{G}_{\lambda_1}, -\Delta\phi_{2,\lambda_2} - \lambda_2 q_2 \mathcal{G}_{\lambda_2}).$$

The boundary conditions in (1.10) can be written as following

$$\begin{cases} \phi_{1,\lambda_1}(0) = -\beta q_2(0) + (\sigma_1 + \theta_{\lambda_1}) q_1. \\ \phi_{2,\lambda_2}(0) = -\beta q_1(0) + (\sigma_2 + \theta_{\lambda_2}) q_2. \end{cases}$$

Finally, we show that the quadratic form $Q : \Lambda \to L^2(\mathcal{I})$ associated with the operator H has domain

$$\Lambda := \mathcal{D} \times \mathcal{D} = \{U = (u_1, u_2) \in L^2(\mathcal{I}) : u_1, u_2 \in \mathcal{D}\},$$

and action

$$Q(U) = Q_{\sigma_1}(u_1) + Q_{\sigma_2}(u_2) - 2\beta \mathrm{Re}\{q_2 \overline{q_1}\}.$$

In particular, the quadratic form Q is symmetric and

$$Q = \langle U, HU \rangle_{L^2(\mathcal{I})}, \qquad \forall U \in \mathcal{D}(H).$$

Remark 1.6.1. It is possible to define the operator H for every $\beta \in \mathbb{C}$; it is sufficient to substitute the condition in (1.10) with the more general condition

$$\begin{pmatrix} \phi_{1,\lambda_1}(0) - \theta_{\lambda_1} q_1 \\ \phi_{2,\lambda_2}(0) - \theta_{\lambda_2} q_2 \end{pmatrix} = \begin{pmatrix} \sigma_1 & -\beta \\ -\overline{\beta} & \sigma_2 \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}$$

Nevertheless, from the variational perspective, without loss of generality we can reduce to the study of the case $\beta \geqslant 0$, as observed in [4].

Chapter 2

Some properties of the Nonlinear Schrödinger Equation

In this chapter, we introduce some relevant features of the Nonlinear Schrödinger equation (NLS) in $\mathbb{R}^n$ [13, 26, 56, 77]. In particular, we will focus first on the time-dependent problem, reporting results about the well-posedness and the conserved quantities, and then on particular stationary solutions called standing waves.

We will consider a nonlinear Schrödinger equation with a power-type nonlinearity, namely

$$i\frac{\partial}{\partial t}\psi = -\Delta\psi + \beta|\psi|^{p-2}\psi, \tag{2.1}$$

where $\beta \in \mathbb{R}$ and $p > 2$.
We note that the NLS equation (2.1) is referred as focusing if $\beta < 0$ and defocusing if $\beta > 0$. The unknown $\psi : \mathbb{R}\times\mathbb{R}^n \to \mathbb{C}$ is a complex valued function of the time $t \in \mathbb{R}$ and of the space $x \in \mathbb{R}^n$ for $n \geq 1$. One important difference between the focusing and defocusing NLS equation is represented by the specific standing waves that the two equations admit. In particular, the focusing NLS equation, corresponding to $\beta < 0$, admits the so-called *bright solitons* (or simply *solitons*), which decays to zero at infinity. On the other hand, for the defocusing NLS equation, corresponding to $\beta > 0$, there exist other type of solutions, called *dark solitons*: such solutions do not vanish at infinity, [66]. For this reason, along this chapter we will deal only with the focusing case.

Well posedness and conservation laws

In this subsection, we will focus on the well-posedness and on the conserved quantities associated with (2.1).

For the physical properties of the equation, it is important to look for quantities that are conserved over time. At least formally, equation (2.1) admits three conserved quantities. The first one is the *mass*: if φ satisfies (2.1) with the initial condition $\varphi(0) = \varphi_0$, then

$$Q(\varphi(t)) := \frac{1}{2}\|\varphi(t)\|^2_{L^2(\mathbb{R}^n)} = Q(\varphi_0).$$

The conservation of the mass is formally derived by multiplying equation (2.1) by $\overline{\varphi}$, integrating over $\mathbb{R}^n$, and taking the imaginary part. The second conserved quantity is the

energy

$$E_p(\varphi(t)) := \frac{1}{2}\|\nabla\varphi(t)\|^2_{L^2(\mathbb{R}^n)} - \frac{1}{p}\|\varphi(t)\|^p_{L^p(\mathbb{R}^n)} = E(\varphi_0).$$

Such conservation law can be obtained by multiplying equation (2.1) by $\partial_t\overline{u}$, integrating over $\mathbb{R}^n$, and taking the real part. Finally, the third conserved quantity is the *momentum,*

$$M(\varphi(t)) := Im\int_{\mathbb{R}^n}\varphi(t)\nabla\overline{\varphi}(t)\,dx = M(\varphi_0).$$

To make these arguments rigorous, it is natural to look for solutions to equation (2.1) in functional spaces where these quantities are well-defined: our choice is to consider $\phi_0 \in H^1(\mathbb{R}^n)$. The next results deals with the local well-posedness of the Cauchy problem, the conservation laws and the blow-up alternative associated with equation (2.1) [26, 27].

Proposition 2.0.1. [27, Proposition 2.1] Let $2 < p < 2 + \frac{4}{n-2}$ if $n \geq 3$ and $2 < p < +\infty$ if $n = 1, 2$. For every $\psi_0 \in H^1(\mathbb{R}^n)$ there exists a unique maximal solution ψ of (2.1) such that $\psi(0) = \psi_0$ and

$$\psi \in C((T_{min}, T^{max}); H^1(\mathbb{R}^n)) \cap C^1((T_{min}, T^{max}); H^{1^*}(\mathbb{R}^n)),$$

where $T_{min} \in [-\infty, 0)$ and $T^{max} \in (0, +\infty]$. Furthermore, the conservation of mass, energy and momentum holds, namely for every $t \in (T_{min}, T^{max})$

$$Q(\psi(t)) = Q(\psi_0),\ E(\psi(t)) = E(\psi_0),\ M(\psi(t)) = M(\psi_0).$$

Finally, we have the blow-up alternative:

1. If $T_{min} > -\infty$, then $\lim_{t\to(T_{min})^+}\|\nabla\psi(t)\|^2_{L^2(\mathbb{R}^n)} = +\infty$
2. If $T_{max} < +\infty$, then $\lim_{t\to(T^{max})^-}\|\nabla\psi(t)\|^2_{L^2(\mathbb{R}^n)} = +\infty$

The following proposition gives an answer to the question of global existence of solutions of (2.1).

Proposition 2.0.2. [27, Proposition 2.2] If $2 < p < 2 + \frac{4}{n}$, then (2.1) is globally well-posed, i.e. for any solution φ given by Proposition 2.2, $T_{min} = -\infty$ and $T^{max} = +\infty$.

Remark 2.0.3. In the statements of Proposition 2.0.1 and Proposition 2.0.2, the two relevant thresholds $2 + \frac{4}{n-2}$ and $2 + \frac{4}{n}$ appear. In the next sections, we will see that these two threshold are strongly connected with Pohozaev identity and Gagliardo-Nirenberg inequality respectively.

The stationary equation: the variational methods

In this subsection, we will deal with standing waves of (2.1) going to zero at infinity: we will focus on the case where $\beta = -1$ (focusing case), since no such solution exists with a nonlinear defocusing term [13]. Let us start defining what we mean by standing waves for the equation (2.1). Standing waves are particular solution to (2.1) that can be written as the product of a function depending only on the position and a phase factor

depending only on the time, namely $\psi(t,x) = e^{i\omega t}\varphi(x)$ for some $\omega \in \mathbb{R}$ and $\varphi(x) \to 0$ as $|x| \to +\infty$. Given a standing wave $\psi(t,x) = e^{i\omega t}\varphi(x)$, then the associated function φ solves the semilinear elliptic equation

$$\begin{cases} \Delta\varphi - \omega\varphi + |\varphi|^{p-2}\varphi = 0, \\ \varphi(x) \to 0 \quad \text{as} \quad |x| \to +\infty. \end{cases} \tag{2.2}$$

When needed, we will use the notation φ_ω in place of φ to stress the fact that φ_ω solves equation (2.2) for that specific value of ω.
The main feature of these special solutions is that their profile remains unchanged under time evolution. This peculiarity arises from a balance between two opposite effects. On the one hand, the dispersive effect of the linear part of (2.1) tends to flatten the solution as the time goes on. On the other hand, the focusing nonlinear term tends to concentrate the solution.

We will now focus on solutions of (2.2) belonging to the space $H^1(\mathbb{R}^n)$. Some variational methods have been used in the literature to study H^1 solutions of (2.2). The first one consists in minimizing the energy functional

$$E_p(v) := \frac{1}{2}\int_{\mathbb{R}^n} |\nabla v|^2\,dx - \frac{1}{p}\int_{\mathbb{R}^n} |v|^p\,dx, \qquad v \in H^1(\mathbb{R}^n),$$

under the constraint of fixed mass, namely

$$M(v) := \int_{\mathbb{R}^n} |v(x)|^2\,dx = \mu > 0.$$

The second method consists instead in minimizing the action functional $S : H^1(\mathbb{R}^n) \to \mathbb{R}$, defined as

$$S(v) := \frac{1}{2}\|\nabla v\|^2_{L^2(\mathbb{R}^n)} + \frac{\omega}{2}\|v\|^2_{L^2(\mathbb{R}^n)} - \frac{1}{p}\|v\|^p_{L^p(\mathbb{R}^n)},$$

among functions belonging to the Nehari manifold

$$N_\omega := \left\{ v \in H^1(\mathbb{R}^n) \setminus \{0\} \,:\, \|\nabla v\|_2^2 + \omega\|v\|_2^2 - \|v\|_p^p = 0 \right\}.$$

Let us observe that both the minimization problems lead to solutions of the stationary equation (2.2). Indeed, both the energy E and the action S are of class C^2 and, given a standing wave $\varphi \in H^1(\mathbb{R}^n)$, the following equations are satisfied

$$E_p'(\varphi) + \omega M'(\varphi) = S'(\varphi) = -\Delta\varphi + \omega\varphi - |\varphi|^{p-1}\varphi = 0.$$

In fact, this is the result of the Lagrange's multiplier Theorem applied to E and S, with the only difference that no additional Lagrange multiplier appears for the action functional. Let us comment also on the role of the parameter ω in the two different variational problems. In the first case, ω is a Lagrange multiplier, while in the second case it is a parameter of the problem itself: the choice of the variational problem depends on the parameter we want to fix, either the mass μ or the frequency ω.

2.0.1 The stationary equation: main results

Let us first observe that solutions of (2.2) exist only if the frequency $\omega > 0$, as stated in the following lemma.

Lemma 2.0.1. *If $\exists\, \omega \in \mathbb{R}$ and $\exists\, \varphi \in H^1(\mathbb{R}^n) \setminus \{0\}$ such that (ω, φ) is solution of (2.2) then $\omega > 0$.*

Instead of a rigorous proof, let us provide an heuristic argument. Since $\varphi \in H^1$, we have $\lim_{|\mathbf{x}|\to\infty} \varphi = 0$. Therefore, in the asymptotic regime $|\mathbf{x}| \to \infty$, the effect of the nonlinear term becomes negligible, and the equation for the standing wave reduces to:

$$-\Delta\varphi_\omega(\mathbf{x}) + \omega\varphi_\omega = 0,$$

it is clear that when $\omega < 0$, the solutions of the previous equation are oscillatory and do not have sufficient decay to be in H^1.

We are now ready to state the Pohozaev identity.

Lemma 2.0.2. *(see [12]). If $\varphi \in H^1(\mathbb{R}^n)$ satisfies (2.2), then the following identity holds:*

$$\|\nabla\varphi\|_2^2 = \frac{n}{p}\left(\frac{p}{2} - 1\right)\|\varphi\|_p^p.$$

Since we are interested in solutions that decay to zero as $|x| \to \infty$, an application of Pohozaev identity implies that there are no solutions of (2.2) in $H^1(\mathbb{R}^n)$ when $p > \frac{2n}{n-2}$: indeed, this is equivalent to verify that the right-hand sides of the Pohozaev identity is strictly positive, namely

$$\begin{cases} 2 < p < +\infty & \text{if } n = 1, 2 \\ 2 < p < 2 + \frac{4}{n-2} & \text{if } n \geq 3. \end{cases} \tag{2.3}$$

Let us observe that such threshold corresponds to upper bound of powers for which local well-posedness holds (see Proposition 2.0.1).

In the next three results, we report important theorems about existence, uniqueness and regularity of positive solutions of equation (2.2).

Theorem 2.0.4. (see [77, Theorem 4.2]). (Existence of a positive solution or ground state) Suppose $n \geqslant 2$ and $p < 2/(n-2)$ (no condition on p if $n = 2$). Equation (2.2) has a positive, spherically symmetric solution $\varphi \in C^2(\mathbb{R}^n)$. In addition, φ and its derivatives up to order 2 have an exponential decay at infinity. This solution minimizes the action, among all $H^1(\mathbb{R}^n)$-solutions of (2.2).

The next result was proven by Kwong in 1989.

Theorem 2.0.5. (see [77, Theorem 4.3]). (Uniqueness of positive solutions) If $2 < p < 2 + \frac{4}{n-2}$, then the positive solution obtained in the previous theorem is unique.

The next result was proven by Gidas, Ni and Nirenberg in 1979. This theorem is stated for a general nonlinearity f and can be applied in our setting by the choice $f(t) = |t|^{p-2}t - \omega t$.

Theorem 2.0.6. (see [77, Theorem 4.4]). Let $\varphi(\mathbf{x})$ be a C^2 positive solution vanishing at infinity of the equation $\Delta\varphi + f(\varphi) = 0$ in $\mathbb{R}^n, n \geqslant 2$, with $f \in C^{1+\mu}(\mathbb{R}^n), \mu > 0$, $f(0) = 0$, and $f'(0) < 0$. Then $\varphi(\mathbf{x})$ is spherically symmetric about some point in $\mathbb{R}^n$ and $\frac{\partial\varphi}{\partial r} < 0$ for $r > 0$, where r is the radial coordinate about that point. Furthermore,

$$\lim_{r\to\infty} r^{(n-1)/2} e^r \varphi(r) = \text{ const } > 0$$

The last result is about the existence of infinitely many solutions of (2.2). It was established by Strauss (1977) and Berestycki and Lions (1983) for a large class of nonlinearities using critical point theory.

Theorem 2.0.7. (see [77, Theorem 4.5]). Under the same hypothesis of the previous theorems, there exists an infinite number of radially symmetric solutions φ_k of class C^2. Each φ_k has exactly k nodes as a function of $|\mathbf{x}| = r$ and decays exponentially at infinity. In addition, $\mathcal{S}(\varphi_k)$ and $|\nabla\varphi_k|_{L^2} \to \infty$ as $k \to \infty$.

Gagliardo-Nirenberg inequalities and optimal costants

A key tool in the study of NLS equation is given by the so-called *Gagliardo-Nirenberg Inequalities*. Let $v \in H^1(\mathbb{R}^n)$, and let p be in the H^1-subcritical regime (2.3). Then

$$\|v\|_p^p \leqslant C\|\nabla v\|_2^{\frac{p-2}{2}n}\|v\|_2^{p+(1-\frac{p}{2})n} \tag{2.4}$$

where C is a positive constant that depends only on p and n.

Let us explain better why inequality (2.4) plays a crucial role in the existence results about NLS equation. In particular, let us consider the minimization problem associated with the energy E_p at fixed mass, namely for fixed $0 < \mu < \infty$ we look for functions $\varphi \in H^1(\mathbb{R}^n)$ with energy equal to

$$\inf_{v\in H^1(\mathbb{R}^n)} \left\{ E_p(v) \mid \|v\|_2^2 = \mu \right\}. \tag{2.5}$$

By applying Gagliardo-Nirenberg inequality (2.4), there results that

$$\begin{aligned} E_p(v) &= \frac{1}{2}\|\nabla v\|_2^2 - \frac{1}{p}\|v\|_p^p \geqslant \frac{1}{2}\|\nabla v\|_2^2 - \frac{C}{p}\mu^{1+\frac{(p-2)(2-n)}{4}}\|\nabla v\|_2^{\frac{p-2}{2}n} \\ &= \frac{1}{2}\|\nabla v\|_2^2 - \alpha\|\nabla v\|_2^{\frac{p-2}{2}n} \end{aligned} \tag{2.6}$$

where $\alpha = \frac{2C}{p}\mu^{1+\frac{(p-2)(2-n)}{4}} > 0$. The function of $\|\nabla v\|_2$ on the right hand-side of (2.6) is bounded from below for every value of the mass if $2 < p < 2 + \frac{4}{n}$, thus for such values of the power the infimum of the energy E_p is finite: this range of powers is called in the literature L^2-subcritical regime.

If $p = 2 + \frac{4}{n}$, i.e. in the so-called L^2-critical case, then this argument holds for small valued of the mass μ only.

On the other hand, if one considers $\varphi \in H^1(\mathbb{R}^n), \mu = \|\varphi\|_2^2$, and performs the transformations $\varphi^\lambda(x) := \lambda^{\frac{n}{2}}\varphi(\lambda x)$, then

$$\left\|\varphi^\lambda\right\|_2^2 = \mu, \quad E(\varphi^\lambda) = \frac{\lambda^2}{2}\|\nabla\varphi\|_2^2 - \frac{\lambda^{\frac{p-2}{2}n}}{p}\|\varphi\|_p^p.$$

Therefore, if $p = 2 + \frac{4}{n}$ and $\mu >> 1$ or $p > 2 + \frac{4}{n}$, i.e. the so-called the L^2-supercritical case, then $\lim_{\lambda\to\infty} E(\varphi^\lambda) = -\infty$, and so the infimum (2.5) is equal to $-\infty$. In such cases, looking for global minimizers of E_p under the mass constraint does not make sense.

Let us come back to the value of the constant C in (2.4). The original proofs of the Gagliardo-Nirenberg inequality only demonstrated the existence of a positive constant C such that the inequality (2.4) holds. Consequently, for this particular value of C, we have that

$$0 < \frac{1}{C} \leq J[v], \tag{2.7}$$

where

$$J(v) = \frac{\|\nabla v\|_2^{\frac{p-2}{2}n}\|v\|_2^{p+(1-\frac{p}{2})n}}{\|v\|_p^p}$$

with $v \in H^1(\mathbb{R}^n)$, $2 < p < \frac{2}{n-2}$. Clearly, if we substitute C with a larger constant, inequalities (2.4) and (2.7) will still hold. However, if we replace C with a smaller constant, these inequalities may no longer hold for all functions f.

Definition 2.0.8 (Optimal constant)**.** The optimal constant $C_{p,n}$ is the smallest positive number for which the Gagliardo-Nirenberg inequality (2.4) holds for all $v \in H^1$. Therefore,

$$\frac{1}{C_{p,n}} = \inf_{\substack{v\in H^1\\ v\neq 0}} J[v].$$

We now present the calculation of the optimal constant $C_{p,n}$ due to Weinstein. If $v \in H^1(\mathbb{R}^n)(\mathbb{R}^n)$, $0 < p < \frac{2}{n-2}$ and $n \geqslant 2$, is the solution of $\Delta v - v + |v|^{p-2}v = 0$, then is given by

$$C_{p,n} = \frac{p}{2}\frac{2(2 + (\frac{p}{2} - 1)(2 - n))^{\frac{n}{2}(\frac{p}{2}-1)-1}}{(\frac{p-2}{2}n)^{\frac{p-2}{4}n}}\frac{1}{\|v\|_2^{p-2}}.$$

$$\mathcal{C}(\varphi, \nabla\varphi) := \frac{1}{2}\|\nabla\varphi\|_2^2 - \frac{1}{p}\|\varphi\|_p^p - \omega_\mu\left(\|\varphi\|_2^2 - \mu\right),$$

where ω_μ is a Lagrange multiplier. Therefore, $\varphi_\mu^{(0)}$ is the solution of

$$\Delta\varphi + |\varphi|^{p-2}\varphi - \omega_\mu\varphi = 0.$$

2.1 NLS Ground state on quantum hybrids

2.1.1 The plane and halfline hybrid

As already observed, quantum hybrids are multidimensional structures on which quantum dynamics can be defined. These structures consist of different manifolds that are joined together in such a way as to support non-trivial dynamics across the entire system. In [4], the existence and properties of the ground states of a nonlinear Schrödinger equation were studied on a manifold called the hybrid plane. This hybrid plane consists of a halfline, with its origin connected to a plane. Let $\mathcal{J}$ be the hybrid obtained gluing together at a point a halfline, identified with $\mathbb{R}^+$, and a plane, identified with $\mathbb{R}^2$.

A function on the hybrid is a pair $U = (u_1, u_2) : \mathcal{J} \to \mathbb{C}$, with $u_1 : \mathbb{R}^+ \to \mathbb{C}$ is the restriction to the halfline and $u_2 : \mathbb{R}^2 \to \mathbb{C}$ the restriction to the plane. Consistently the Hilbert space for this hybrid will be $L^2(\mathcal{J}) := L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^2)$.
We are interested in the existence of standing waves $\Psi(t, x, \mathbf{x}) = e^{i\omega}U(x, \mathbf{x})$, with $x \in \mathbb{R}^+, \mathbf{x} \in \mathbb{R}^2$, of the equation

$$i\frac{\partial}{\partial t}\Psi = H_{\mathcal{J}}\Psi + \widehat{g}(\Psi),$$

where $\widehat{g} : \mathbb{C}^2 \to \mathbb{C}^2$ is a nonlinear function given by

$$\widehat{g}(z, w) = (-|z|^{p_1-2}z, -|w|^{p_2-2}w), \qquad 2 < p_1 < 6,\ 2 < p_2 < 4.$$

The study of stationary solutions for nonlinear Schrödinger equations on halfline–plane and line–plane hybrids, with power-like focusing and subcritical nonlinearity, is detailed in [4, 5]. These investigations examine the existence, nonexistence, and characteristics of ground states on such hybrid manifolds, which consist of a halfline or a line connected at a point to a plane. The research provides insights into how the interplay between different spatial dimensions influences the behavior of solutions in these nonlinear systems. Given a standing wave $\Psi(t, x, \mathbf{x}) = e^{i\omega}U(x, \mathbf{x})$, with $x \in \mathbb{R}^+, \mathbf{x} \in \mathbb{R}^2$, then the associated function U solves the semi-linear elliptic equation

$$\begin{cases} H_{\mathcal{J}}U + \widehat{g}(U) + \omega U = 0 \\ U \in \mathcal{D}(H_{\mathcal{J}}). \end{cases}$$

Let us highlight that ground states U of the NLS energy functional of the hybrid $\mathcal{J}$, defined as following

$$\widehat{F}(U) := \frac{1}{2}Q_{\mathcal{J}}(U) - \frac{1}{p_1}\int_{\mathbb{R}^+} |u_1|^{p_1}\,dx - \frac{1}{p_2}\int_{\mathbb{R}^2} |u_2|^{p_2}\,dx,$$

remember that

$$Q_{\mathcal{J}}(U) := Q_\alpha(u_1) + Q_\sigma(u_2) - 2\beta\mathrm{Re}\{q\overline{u_1(0)}\}$$

where Q_α and Q_σ are the quadratic forms associated with the operators H_1^α, H_2^σ and $\beta\mathrm{Re}\{q\overline{u_1(0)}\}$ accounts for the coupling between the halfline and the plane.
Let us observe that the energy functional is constructed by considering the contributions from each component of $\mathcal{J}$ (e.g., the halfline and the plane).

$$\widehat{F}(U) = \frac{1}{2}Q_\alpha(u_1) + \frac{1}{2}Q_\sigma(u_2) - \beta\mathrm{Re}\{q\overline{u_1(0)}\} - \frac{1}{p_1}\|u_1\|^{p_1}_{L^{p_1}(\mathbb{R}^+)} - \frac{1}{p_2}\|u_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)}$$

i.e

$$\widehat{F}(U) = F_{p_1,\alpha}(u_1) + F_{p_2,\sigma}(u_2) - \beta \mathrm{Re}\{q\overline{u_1(0)}\}. \tag{2.8}$$

where

$$F_{p_1,\alpha}(u_1) := \frac{1}{2}Q_\alpha(u_1) - \frac{1}{p_1}\|u\|^{p_1}_{L^{p_1}(\mathbb{R}^+)}, \qquad u_1 \in H^1(\mathbb{R}^+) \tag{2.9}$$

and

$$F_{p_2,\sigma}(u_2) = \frac{1}{2}Q_\sigma(u_2) - \frac{1}{p_2}\|u_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)}, \qquad u_2 \in \mathcal{D}. \tag{2.10}$$

The gluing condition at the connecting point introduces additional constraints, ensuring the continuity of the wavefunction and its flux across the interface.
The hybridization process must introduce non-trivial dynamics on the hybrid, meaning dynamic processes that are not simply the juxtaposition of the free dynamics of the separate elements but instead pertain to the entire hybrid, potentially highlighting its geometric peculiarities or the specifics of the gluing conditions.
In the case of nonlinear dynamics, it seems natural to seek a characterization of ground-state solutions influenced by the peculiarities of the hybrid. Moreover, it is necessary that the "zoology" of ground states turns out to be richer than those that can exist individually on the separate components. Let us now introduce the definition of ground states.

Definition 2.1.1 (Ground state)**.** For every fixed $\mu > 0$, we call *ground state* of $\widehat{F}$ at mass $\mu > 0$ any function U belonging to

$$\widehat{\Lambda}_\mu := \left\{ U \in \widehat{\Lambda} : \|U\|^2_{L^2(\mathcal{J})} = \mu \right\},$$

such that

$$\widehat{F}(U) = \widehat{\mathcal{F}}(\mu) := \inf_{U \in \widehat{\Lambda}_\mu} \widehat{F}(U).$$

Finally, $\widehat{\mathcal{F}}$ is called *the energy level of the ground state* of $\widehat{F}$ at mass μ.

Analogously, denote by

$$\mathcal{F}_{p_1,\alpha}(\mu) := \inf_{u_1 \in H^1_\mu(\mathbb{R}^+)} F_{p_1,\alpha}(u_1)$$

and

$$\mathcal{F}_{p_2,\sigma}(\mu) := \inf_{u_2 \in \mathcal{D}} F_{p_2,\sigma}(u_2)$$

the ground-state energy levels of (2.9) and (2.10), respectively. The problem of finding and characterizing the ground states for (2.9) and (2.10) was solved in [2] and [4]. We note that these results are strictly necessary for the forthcoming discussion of the ground state on the full hybrid (see [4, 5]).

In the energy functional, there are two different nonlinearity powers, p_1 and p_2 respectively on the halfline and the plane, to enclose a larger spectrum of problems and to cover

all subcritical cases. In [4] are investigated existence and properties of ground states at fixed mass when both the matrix of the boundary values for the interaction

$$\Sigma = \begin{pmatrix} \alpha & -\beta \\ -\beta & \sigma \end{pmatrix} \in M_{2\times 2}$$

and the powers of the nonlinearities $p_1 \in (2,6)$ and $p_2 \in (2,4)$ vary.

If consider a ground state $U = (u_1, u_2)$, then $u_1 \in H^2(\mathbb{R}^+)$, $\phi_\lambda := u_2 - q\mathcal{G}_\lambda \in H^2(\mathbb{R}^2)$ for some $\lambda > 0$ and they have to verify for some $\omega \in \mathbb{R}$ the system

$$\begin{cases} -u_1'' + \omega u_1 - |u_1|^{p_1-2}u_1 = 0, \\ -\Delta\phi_\lambda + \omega\phi_\lambda + (\omega - \phi_\lambda)q\mathcal{G}_\lambda - |u_2|^{p_2-2}v = 0, \\ u_1'(0) = \alpha u_1(0) - \beta q, \\ \phi_\lambda(0) = -\beta u_1(0) + (\sigma + \theta_\lambda q). \end{cases}$$

The first result of existence is presented in [4, Theorem 1]. Before stating it, we introduce some useful objects. First of all, we define the function

$$\mathcal{E}_p(\mu, X) = \inf_{u\in H^1_\mu(X)} E_p(u, X), \qquad \mu > 0,$$

with $X = \mathbb{R}^n$, $n = 1, 2$. If clear from the context, we will not specify the dependence on X. More precisely, for each μ we have:

1. If we denote φ_μ the unique and even ground state a mass μ of the energy functional with $X = \mathbb{R}$, we have that

$$E_{p_1}(\varphi_\mu) = -\mathcal{E}_{p_1}(1)\mu^{\frac{p_1+2}{6-p_1}}, \qquad \mathcal{E}_{p_1}(1) < 0$$

2. Analogously, denote by ϕ_μ the unique positive and spherically symmetric ground state at mass μ of the energy functional with $X = \mathbb{R}^2$, we have that

$$E_{p_2}(\phi_\mu) = -\mathcal{E}_{p_2}(1)\mu^{\frac{2}{4-p_2}}, \qquad \mathcal{E}_{p_2}(1) < 0$$

We are now ready to state the necessary and sufficient condition for the existence of ground states.

Theorem 2.1.2. ([4, Theorem 1]) A ground state at mass μ for the energy (2.8) on the hybrid plane $\mathcal{J}$ exists if and only if there is a function $U \in \widehat{\Lambda}_\mu$ such that

$$\widehat{F}(U) \le E_{p_1}(\varphi_\mu) = \mathcal{E}_{p_1}(1)\mu^{\frac{p_1+2}{6-p_1}}.$$

where φ_μ is a ground state at mass μ for the standard NLS energy $E_{p_1}(\cdot, \mathbb{R})$.

Before going on with the statements of the other results, let us explain why the energy of the soliton on the real line $E_{p_1}(\varphi_\mu)$ plays a crucial role. To do this, let us illustrate the general arguments that lead to this result.
The first step is the proof of the coercivity of the functional energy (2.8) on $\widehat{\Lambda}_\mu$, for that we will us two different Gagliardo-Nirenberg inequalities:

1. A standard one dimensional Gagliardo-Nirenberg inequality for the halfline: for all $p_1 \in (2, +\infty]$
$$\|u_1\|_{L^{p_1}(\mathbb{R}^+)} \leqslant K \|u_1'\|_{L^2(\mathbb{R}^+)}^{\frac{p_1-2}{2p_1}} \|u_1\|_{L^2(\mathbb{R}^+)}^{\frac{p_1+2}{2p_1}};$$

2. modified two dimensional Gagliardo-Nirenberg inequality [7] for the plane: for all $p_2 \in (2, +\infty)$ and $M > 0$, recalling $u_2 = \phi_{\lambda(u)} + q\mathcal{G}_{\lambda(u)} \in \mathcal{D} \setminus H^1(\mathbb{R}^2)$, with $\lambda(u) = |q|/\|u\|_2^2$, satisfies
$$\|u_2\|_{L^{p_2}(\mathbb{R}^2)}^{p_2} \leqslant M \left(\|\nabla \phi_{\lambda(u)}\|_{L^2(\mathbb{R}^2)}^{p_2-2} + |q|^{p_2-2} \right) \|u_2\|_{L^2(\mathbb{R}^2)}^2. \tag{2.11}$$

The second step consists in considering a minimizing sequence U_k, i.e. $U_k = (u_k, v_k) \in \widehat{\Lambda}_\mu$ such that $\widehat{F}(U_k) \to \widehat{\mathcal{F}}(\mu)$. By exploiting Gagliardo-Nirenberg inequalities it is easy to show that $U_k \rightharpoonup U$ in $\widehat{\Lambda}$. Then, by using Brezis-Lieb lemma, sub-additivity of $\widehat{\mathcal{F}}(\mu)$ and (2.11), we can conclude that U is a ground state whenever $\|U\|_{L^2(\mathcal{J})} \neq 0$.

Therefore, the problem is reduced to study the conditions for which $\|U\|_{L^2(\mathcal{J})} = 0$ holds. The condition $\|U\|_{L^2(\mathcal{I})} = 0$ can be realized when $u_k \to 0$ in $L^{p_1}(\mathbb{R}^+)$ and $v_k \to 0$ in $L^{p_2}(\mathbb{R}^2)$. This condition is not compatible and it generates a contradiction.
The condition $\|U\|_{L^2(\mathcal{I})} = 0$ can be realized also when $u_k \to 0$ in $L^{p_1}_{\mathrm{loc}}(\mathbb{R}^+)$ and $v_k \to 0$ in $L^{p_2}_{\mathrm{loc}}(\mathbb{R}^2)$, but either $u_k \not\to 0$ in $L^{p_1}(\mathbb{R}^+)$ or $v_k \not\to 0$ in $L^{p_2}(\mathbb{R}^2)$. This situation is related to the following situations: $(u_k)_k$ runs away on the halfline and $(v_k)_k$ vanishes; $(v_k)_k$ runs away on the plane and $(u_k)_k$ vanishes. In the first case we have that

$$\widehat{\mathcal{F}}(\mu) \approx \mathcal{E}_{p_1}(\mu, \mathbb{R}),$$

while, in the second case, we have that

$$\widehat{\mathcal{F}}(\mu) \approx \mathcal{E}_{p_2}(\mu, \mathbb{R}^2).$$

If we find a state U such that $\widehat{\mathcal{F}}(\mu) < \min\{\mathcal{E}_{p_1}(\mu, \mathbb{R}^+), \mathcal{E}_{p_2}(\mu, \mathbb{R}^2)\}$, then we get that U is a ground state of $\widehat{F}$ at mass μ.
Since $\widehat{F}_{|H^1(\mathbb{R}^+)\oplus\{0\}} = F_{p_1,\alpha}(\cdot, \mathbb{R}^+)$ and $\widehat{F}_{|\{0\}\oplus\mathcal{D}} = F_{p_2,\sigma}(\cdot, \mathbb{R}^2)$, there results that

$$\widehat{\mathcal{F}}(\mu) \leqslant \min\left\{\mathcal{F}_{p_1,\alpha}(\mu), \mathcal{F}_{p_2,\sigma}(\mu)\right\}.$$

By [7], we have $\mathcal{F}_{p_2,\sigma}(\mu) < \mathcal{E}_{p_2}(\mu)$, thus the criterion for the existence of ground states can be simplified, reducing to the comparison with the energy of the one-dimensional soliton $E_{p_1}(\varphi_\mu)$.

The first consequence of this theorem (see [4], Corollaries 2.2 and 2.4) is that for every choice of the parameters $\alpha \in \mathbb{R}$, $p_1 \in (2, 6)$ a ground state exists for small and for large mass. This result is obtained through an asymptotic analysis and does not provide relevant estimates of mass thresholds. The second consequence of Theorem 2.1.2 is that

$$\mathcal{E}_{p_2}(1)\mu^{\frac{p_2+2}{6-p_2}} < \mathcal{E}_{p_1}(1)\mu^{\frac{2}{4-p_1}}, \tag{2.12}$$

and gives for the mass the threshold value

$$\mu_{p_1,p_2} = \left(\frac{\mathcal{E}_{p_1}(1)}{\mathcal{E}_{p_2}(1)}\right)^{\frac{p_1p_2-4p_1-6p_2+24}{6p_1-2p_2-p_1p_2-4}}.$$

Since the exponent on the left of (2.12) is smaller that the exponent at the right if only if

$$p_1 > r^\star = \frac{6p_1-4}{p_1+2}.$$

These are given in the next corollary.

Corollary 2.1.3. ([4, Corollary 2.3]) Fix $p_1 \in (2,6)$, $p_2 \in (2,4)$. If

$$\begin{gathered} p_2 < r^\star \text{ and } \mu \in (0, \mu_{p_1,p_2}] \\ \text{or} \\ p_2 > r^\star \text{ and } \mu \geq \mu_{p_1,p_2} \end{gathered} \tag{2.13}$$

then there is a ground state at mass μ for the energy (2.8).

The last corollary shows that for fixed μ the existence of a ground state mass μ is ensured if α is negative or sufficiently small with respect to μ.

Corollary 2.1.4. ([4, Corollary 2.5]) For any $\mu > 0$ and $p \in (2,6)$ there is a number $\alpha_p > 0$ such that, if

$$\begin{gathered} \alpha < \alpha_p(\mu) \\ \text{or} \\ \alpha = \alpha_p(\mu) \text{ and } 2 < p < 6 \end{gathered} \tag{2.14}$$

then there exists a ground state at mass μ for the energy (2.8).

Finally, if we are not in the hypotheses of previous three corollaries that guarantee existence, then there are no ground states, as stated in the next theorem.

Theorem 2.1.5. ([4, Theorem 2]) Let $p_1 \in (2,6)$, $p_2 \in (2,4) \setminus \{r^\star\}$, $\mu > 0$. Assume also that (2.13) does not hold and (2.14) holds. There exists $\rho^\star(r,p,\mu) \in \mathbb{R}$ such that:

i) if $\beta = 0$, then ground states at mass μ for the energy (2.8) do not exist if and only if $\rho > \rho^\star$;

ii) if $\beta > 0$ and $\alpha \neq \alpha_p(\mu)$, setting

$$k^\star := \frac{\beta^2}{\alpha - \alpha_p(\mu)},$$

then ground states at mass μ for the energy (2.8) exists when $\rho \leq \rho^\star$ and do not exist when $\rho > \rho^\star + k^\star$ or $\rho = \rho^\star + k^\star$ and $p \in (2,4]$.

Chapter 3

Normalized NLS ground states on a double plane hybrid

The main goal is to study the existence and the properties of particular solutions of (3.1), namely ground states of the energy associated with (3.1) subject to the constraint of fixed L^2 norm. The precise definition of the energy and of ground states is not straightforward and requires to be introduced step by step.

3.1 The problem

We investigate the existence and the properties of normalized ground states of a nonlinear Schrödinger equation on a quantum hybrid formed by two planes connected at a point. The nonlinearities are of power type and L^2-subcritical, while the matching condition between the two planes generates two point interactions of different strengths on each plane, together with a coupling condition between the two planes. We prove that ground states exist for every value of the mass and two different qualitative situations are possible depending on the matching condition: either ground states concentrate on one of the plane only, or ground states distribute on both the planes and are positive, radially symmetric, decreasing and present a logarithmic singularity at the origin of each plane. Moreover, we discuss how the mass distributes on the two planes and compare the strengths of the logarithmic singularities on the two planes when the parameters of the matching condition and the powers of the nonlinear terms vary.
This chapter of the thesis continues the investigation of stationary solutions of nonlinear Schrödinger equations on quantum hybrids: the first results of this kind have been briefly presented in Section 2.1, where a plane + halfline hybrid and a plane + line hybryd were considered. Here we consider instead a double plane hybrid, namely a hybrid structure where two identical planes are connected at a single point. The dynamics is described, as we have already seen in the introduction, by a nonlinear Schrödinger equation of the form

$$i\frac{\partial}{\partial t}\Psi = H\Psi + g(\Psi), \qquad \Psi = (z,w) : L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2) \to \mathbb{C}^2 \tag{3.1}$$

where $g : \mathbb{C}^2 \to \mathbb{C}^2$ is a nonlinear function given by

$$g(z,w) = (-|z|^{p_1-2}z, -|w|^{p_2-2}w), \qquad p_1, p_2 > 2$$

and H is a self-adjoint operator on the quantum hybrid $\mathcal{I}$. Such a dynamics coincides with the standard NLS dynamics on each plane far from the points where the planes are glued together and allow a connection between the two planes through proper matching conditions that make the operator H a self-adjoint operator. Given a standing wave $\Psi(t,x,y) = e^{i\omega}U(x,y)$, with $x,y \in \mathbb{R}^2$, then the associated function $U(x,y)$ solves

$$\begin{cases} H\,U + g(U) + \omega U = 0 \\ U \in \mathcal{D}(H). \end{cases} \tag{3.2}$$

In order to introduce precisely the problem on the hybrid, we start recalling the definition of the standard NLS energy on the plane, that is

$$E_p(u) := \frac{1}{2}\int_{\mathbb{R}^2} |\nabla u|^2\,dx - \frac{1}{p}\int_{\mathbb{R}^2} |u|^p\,dx, \qquad u \in H^1(\mathbb{R}^2),$$

and suppose that the energy on the hybrid presents an interaction between the two planes that is concentrated only at the junction point: this interaction produces a point interaction on each plane together with a coupling term between the two planes. We have already observed in Chapter 2 that the point interaction on each plane can be defined through the theory of self-adjoint extensions of hermitian operators introduced by Krein and Von Neumann (see [47]) and produces a peculiar decomposition of the energy domain $\mathcal{D}$, namely every function $u \in \mathcal{D}$ decomposes as the sum of a *regular part* $\phi \in H^1(\mathbb{R}^2)$ and a *singular part* $q\mathcal{G}_1$, where $q \in \mathbb{C}$ is usually called the *charge* and $\mathcal{G}_1$ is the Green's function of $-\Delta + 1$: more specifically, $\mathcal{D}$ reads as

$$\mathcal{D} := \{u \in L^2(\mathbb{R}^2) : \exists\, q \in \mathbb{C} \,:\, u - q\mathcal{G}_1 := \phi \in H^1(\mathbb{R}^2)\}.$$

The NLS energy with point interaction on the plane is thus defined as the functional $F_{p,\sigma} : \mathcal{D} \to \mathbb{R}$ acting as

$$\begin{aligned} F_{p,\sigma}(u) :=& \frac{1}{2}Q_\sigma(u) - \frac{1}{p}\|u\|^p_{L^p(\mathbb{R}^2)} \\ =& \frac{1}{2}\left(\|\phi\|^2_{H^1(\mathbb{R}^2)} - \|u\|^2_{L^2(\mathbb{R}^2)}\right) + \frac{|q|^2}{2}\left(\sigma + \frac{\gamma - \log(2)}{2\pi}\right) - \frac{1}{p}\|u\|^p_{L^p(\mathbb{R}^2)}, \end{aligned} \tag{3.3}$$

with γ being the Euler-Mascheroni constant. The parameter σ, later referred as the parameter of the point interaction, is obtained by applying the technique of self-adjoint extension of symmetric operators to the Laplace operator $-\Delta$ on $C_c^\infty(\mathbb{R}^2 \setminus \{0\})$. Let us observe that the value of the parameter σ for which the standard NLS energy is recovered is formally given by $\sigma = +\infty$: indeed, this choice forces the charge q to be zero, so that the domain $\mathcal{D}$ reduces to $H^1(\mathbb{R}^2)$. The existence and some stability properties of the ground states of the energy (3.3) have been studied in [3, 39] and, in presence of a nonlocal nonlinearity, in [40]. Moreover, well-posedness, scattering properties and blow-up of solutions of the associated nonlinear Schrödinger equation have been investigated in [25, 24, 37].

Given $p_i > 2$, $\sigma_i \in \mathbb{R}$ for $i = 1,2$ and $\beta \geqslant 0$, and denoted by $U = (u_1, u_2) \in \Lambda := \mathcal{D} \times \mathcal{D}$ and by $q_i := \lim_{|x|\to 0} \frac{u_i(x)}{\mathcal{G}_1(x)}$ the charges associated with u_i for $i = 1,2$, one can define the

NLS energy on the double-plane hybrid as the functional $F : \Lambda \to \mathbb{R}$ acting as

$$F(U) := \sum_{i=1,2} F_{p_i,\sigma_i}(u_i) - \beta \mathrm{Re}\{q_1 \overline{q_2}\}. \tag{3.4}$$

As one can notice, the coupling term is chosen to be quadratic as function of the charges q_i: by this choice, the operator associated with the quadratic part of the energy turns out to be self-adjoint (see Section 2.1). Let us observe that, denoted with

$$Q(U) := \sum_{i=1,2} Q_{\sigma_i}(u_i) - 2\beta \mathrm{Re}\{q_1 \overline{q_2}\},$$

then the energy (3.4) can be rewritten also as

$$F(U) = \frac{1}{2} Q(U) - \sum_{i=1,2} \frac{1}{p_i} \|u_i\|^{p_i}_{L^{p_i}(\mathbb{R}^2)}.$$

Let us now give the definition of ground state.

Definition 3.1.1. (Ground state). For every fixed $\mu > 0$, we call *ground state* of F at mass μ any function U belonging to

$$\Lambda_\mu := \left\{ (u_1, u_2) \in \Lambda \,:\, \|u_1\|^2_{L^2(\mathbb{R}^2)} + \|u_2\|^2_{L^2(\mathbb{R}^2)} = \mu \right\}$$

such that

$$F(U) = \mathcal{F}(\mu) := \inf_{U \in \Lambda_\mu} F(U)$$

In particular, $\mathcal{F}(\mu)$ is called *ground state energy level* of F at mass μ.

Let us highlight that ground states U of energy functional of the double plane hybrid, (3.4), at mass μ solve for some $\omega \in \mathbb{R}$ the system (3.2). Given a solution of (3.2), one can construct *standing wave* solution of (1.1). Equation (3.2) can thus be rewritten as

$$\begin{cases} (-\Delta + \omega)\phi_{i,\lambda_i} + (\omega - \lambda_i) q_i \, \mathcal{G}_{\lambda_i} - |u_i|^{p_i - 2} u_i = 0, \quad i = 1, 2, \\ \phi_{1,\lambda_1}(0) = (\sigma_1 + \theta_{\lambda_1}) q_1 - \beta q_2, \\ \phi_{2,\lambda_2}(0) = -\beta q_1 + (\sigma_2 + \theta_{\lambda_2}) q_2. \end{cases} \tag{3.5}$$

Summing up, we investigate the following problem:

Problem. Given $p_i \in (2, 4)$, $\sigma_i \in \mathbb{R}$ for $i = 1, 2$, $\beta \geqslant 0$ and $\mu > 0$, study the existence and qualitative properties of ground states at mass μ of the energy (3.4), namely minimizers of

$$\begin{aligned} F(U) &= \sum_{i=1,2} F_{p_i,\sigma_i}(u_i) - \beta \mathrm{Re}\{q_1 \overline{q_2}\} = \\ &= \sum_{i=1,2} \left\{ \frac{1}{2} Q_{\sigma_i}(u_i) - \frac{1}{p_i} \|u_i\|^{p_i}_{L^{p_i}} \right\} - \beta \mathrm{Re}\{q_1 \overline{q_2}\} \end{aligned}$$

among all the functions belonging to Λ_μ.

Let us highlight that the limitations on the values of the powers p_i for $i = 1, 2$ reduce the study to the L^2-subcritical case, namely the case where the energy F is bounded from below for every value of the mass $\mu > 0$: this can be proved in general by applying the so-called Gagliardo-Nirenberg type inequalities (see Subsection 3.3.3).

In order to ease the notation, in the following we will often use F_i in place of F_{p_i,σ_i}. Moreover, we will denote the ground state energy levels of E_p and F_i at mass μ respectively as

$$\mathcal{E}_p(\mu) := \inf_{v \in H^1_\mu(\mathbb{R}^2)} E_p(v)$$

and

$$\mathcal{F}_i(\mu) := \inf_{v \in \mathcal{D}_\mu} F_i(v), \quad i = 1, 2,$$

where the subscript μ in $H^1(\mathbb{R}^2)$ and $\mathcal{D}$ denotes that the additional constraint $\|v\|^2_{L^2(\mathbb{R}^2)} = \mu$ holds.

3.2 Main results

We present now the main results of the paper. We recall that the parameters in (3.4) are chosen as follows when not specified: $p_i \in (2, 4)$, $\sigma_i \in \mathbb{R}$ for $i = 1, 2$, and $\beta \geqslant 0$.
The first result concerns the existence of ground states at fixed mass.

Theorem 3.2.1 (Existence of ground states)**.** For every $\mu > 0$, there exists at least a ground state of (3.4) at mass μ.

Differently from the case of other hybrids considered [4, 5], ground states exist for every value of the mass when two planes are connected at a single point. This is due to the fact that point interactions on the plane are always attractive, namely the associated self-adjoint operators on the plane have always a negative eigenvalue, and this makes more convenient to concentrate around the point of contact rather than escaping at infinity.

In the second result, we provide a characterization of ground states at fixed mass both when $\beta = 0$ and $\beta > 0$. These two cases correspond to the decoupled and coupled case respectively and are coherent with what happens in the linear setting [36], in the sense that the actual hybridization of the two planes happen when the coupling parameter β is different from zero.

Theorem 3.2.2. Let $\mu > 0$. If $\beta = 0$, then

$$\mathcal{F}(\mu) = \min\left\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\right\}. \tag{3.6}$$

Moreover, every ground state U is of the form

i) $U = (u_1, 0)$, if $\mathcal{F}_1(\mu) < \mathcal{F}_2(\mu)$;

ii) $U = (0, u_2)$, if $\mathcal{F}_1(\mu) > \mathcal{F}_2(\mu)$;

iii) either $U = (u_1, 0)$ or $U = (0, u_2)$, if $\mathcal{F}_1(\mu) = \mathcal{F}_2(\mu)$,

and the non-zero component of U is positive, radially symmetric and decreasing along the radial direction and has positive charge, up to a multiplication by a phase factor.

If instead $\beta > 0$, then

$$\mathcal{F}(\mu) < \min\left\{\mathcal{F}_1(\mu)\,,\,\mathcal{F}_2(\mu)\right\}. \tag{3.7}$$

In particular, given $U = (u_1, u_2)$ a ground state of F at mass μ and q_i be the charge associated with u_i, then, up to a multiplication by a phase factor, $q_i > 0$ and u_i is positive, radially symmetric and decreasing along the radial direction for $i = 1, 2$. Furthermore, denoted by ω the Lagrange multiplier associated with U, by $\mathcal{G}_\omega$ the Green's function of $-\Delta + \omega$ and by $\phi_{i,\omega} := u_i - q_i\mathcal{G}_\omega$ for $i = 1, 2$, then also $\phi_{i,\omega}$ is positive, radially symmetric and decreasing along the radial direction.

Remark 3.2.3. As explained in Subsection 3.3.1, the decomposition consider in Theorem 3.2.2, i.e $u_i = \phi_{i,\omega} + q_i\mathcal{G}_\omega$, is another possible decomposition for u_i, that differs from the one presented in the Introduction from the fact that the singular term is given by the Green's function of $-\Delta + \omega$ instead of the Green's function of $-\Delta + 1$.

In the next result, we investigate the distribution of the charges and of the mass on the hybrid when the parameter of the point interaction on the first plane is lower than the same parameter on the second plane and the power nonlinearities are the same on each plane.

Theorem 3.2.4. Let $\sigma_1 < \sigma_2$, $\beta > 0$ and $p_1 = p_2$ and let $U = (u_1, u_2)$ be a ground state of (3.4) at mass $\mu > 0$. For $i = 1, 2$, denote by q_i the charge associated with u_i and by μ_i the mass of u_i. Therefore, it holds that

i) $q_2 < q_1$;

ii) for any $\sigma_1 \in \mathbb{R}$ and $\sigma_2 \to +\infty$, it holds that

$$\|u_1\|^2_{L^2(\mathbb{R}^2)} \to \mu \quad \text{and} \quad F(U) \to \mathcal{F}_1(\mu);$$

In the last theorem, we investigate the distribution of mass on the hybrid when the parameters of the point interactions on the two planes are equal and sufficiently large and the power nonlinearity on the first plane is smaller than the one on the second. Before stating the result, let us introduce for every $p_1 \neq p_2$ the critical mass

$$\mu^\star := \left(\frac{\mathcal{E}_{p_1}(1)}{\mathcal{E}_{p_2}(1)}\right)^{\frac{(4-p_1)(4-p_2)}{2(p_2-p_1)}}. \tag{3.8}$$

Theorem 3.2.5. Let $\sigma_1 = \sigma_2 = \sigma$, $p_1 < p_2$, $\mu > 0$ and $U = (u_1, u_2)$ be a ground state of F at mass $\mu > 0$. Then, as $\sigma \to +\infty$, the following limits hold:

i) if $\mu < \mu^\star$, then

$$\|u_1\|^2_{L^2(\mathbb{R}^2)} \to \mu \quad \text{and} \quad F(U) \to \mathcal{E}_{p_1}(\mu),$$

ii) if $\mu > \mu^\star$, then

$$\|u_2\|^2_{L^2(\mathbb{R}^2)} \to \mu \quad \text{and} \quad F(U) \to \mathcal{E}_{p_2}(\mu).$$

Theorem 3.2.5 and Theorem 3.2.4 are the first results on the distribution of the mass and of the charges on a quantum hybrid. The results are obtained in some specific regimes of the parameters only, and this is due to technical reasons. One of the main obstacle is due to the presence of the point interaction, that breaks the invariance by dilations of the equation and does not allow to perform the standard scalings associated with the Nonlinear Schrödinger Equation. Therefore, it becomes difficult to obtain precise informations on the infimum of the NLS energy with point interaction as function of the mass and the other parameters, and this seems a crucial ingredient to understand the problem in more generality.

3.3 Well-known facts and results

In this section, we recall some preliminary results, in particular concerning the domain of the energy with point interaction in Subsection 3.3.1, the problem at infinity on the hybrid in Subsection 3.3.2 and Gagliardo-Nirenberg inequalities in Subsection 3.3.3;

3.3.1 About the representation of the domain $\mathcal{D}$

First of all, let us recall that every function $u \in \mathcal{D}$ can be written as the sum of a *regular part* belonging to $H^1(\mathbb{R}^2)$ and a *singular part* given by a complex multiple of $\mathcal{G}_1$, which is the Green's function of $-\Delta + 1$. This representation is only one possible way to represent functions in $\mathcal{D}$. Indeed, if one denotes by $\mathcal{G}_\lambda$ the Green's function of $-\Delta + \lambda$ for any $\lambda > 0$, then one can write u as

$$u = \phi_\lambda + q\mathcal{G}_\lambda, \quad \text{with} \quad \phi_\lambda := \phi + q\left(\mathcal{G}_1 - \mathcal{G}_\lambda\right) \in H^1(\mathbb{R}^2).$$

Moreover, it is not hard to see that the quadratic form Q_σ can be written as function of ϕ_λ and q as

$$Q_\sigma(u) = \|\nabla\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} + \lambda\|\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} - \lambda\|u\|^2_{L^2(\mathbb{R}^2)} + |q|^2\left(\sigma + \theta_\lambda\right),$$

with

$$\theta_\lambda := \frac{\log(\sqrt{\lambda}/2) + \gamma}{2\pi}.$$

Therefore, the domain and the action of the energy $F_{p,\sigma}$ can be written respectively as

$$\mathcal{D} = \{u \in L^2(\mathbb{R}^2) \,:\, \exists\, q \in \mathbb{C}, \lambda > 0 : u - q\mathcal{G}_\lambda := \phi_\lambda \in H^1(\mathbb{R}^2)\}$$

and

$$F_{p,\sigma}(u) = \frac{1}{2}\left(\|\nabla\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} + \lambda\|\phi_\lambda\|^2_{L^2(\mathbb{R}^2)} - \lambda\|u\|^2_{L^2(\mathbb{R}^2)}\right) + \frac{|q|^2}{2}\left(\sigma + \theta_\lambda\right) - \frac{1}{p}\|u\|^p_{L^p(\mathbb{R}^2)}.$$

This alternative way of representing functions belonging to $\mathcal{D}$ is very important in some of the proofs of the paper (see for example Theorem 3.2.1).

3.3.2 The problem at infinity on the hybrid.

Particularly relevant in such minimization problems is the so-called problem at infinity.

Let us consider the energy $F^\infty : H^1(\mathbb{R}^2) \times H^1(\mathbb{R}^2) \to \mathbb{R}$, defined as

$$F^\infty(U) := E_{p_1}(u_1) + E_{p_2}(u_2),$$

and the associated ground states energy level

$$\mathcal{F}^\infty(\mu) := \inf_{\substack{U \in H^1(\mathbb{R}^2)\times H^1(\mathbb{R}^2) \\ \|U\|_2^2 = \mu}} F^\infty(U). \tag{3.9}$$

In the next lemma, we provide a first characterization of (3.9) when $p_i \in (2,4)$.

Lemma 3.3.1. *Let $p_i \in (2,4)$ for $i = 1,2$. Then for every $\mu > 0$*

$$\mathcal{F}^\infty(\mu) = \min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\}.$$

Proof. Let us first observe that the minimization problem (3.9) is decoupled and can be reduced to an algebraic problem, in particular

$$\mathcal{F}^\infty(\mu) = \inf\{\mathcal{E}_{p_1}(\mu_1) + \mathcal{E}_{p_2}(\mu_2) : \mu_1 + \mu_2 = \mu\}.$$

It is well known that $\mathcal{E}_p(\mu) < 0$ for every $\mu > 0$ and $p > 2$ and $\mathcal{E}_p(\mu) > -\infty$ for every $\mu > 0$ and p belonging to the L^2-subcritical regime, i.e. $2 < p < 4$. Moreover, by scaling properties of the energy, it follows that $\mathcal{E}_p(\mu) = -\rho_p \mu^{\frac{2}{4-p}}$, with $\rho_p = -\mathcal{E}_p(1)$, thus

$$\mathcal{F}^\infty(\mu) = \inf_{m \in [0,\mu]} g(m),$$

where

$$g(m) = -\rho_{p_1}\, m^{\frac{2}{4-p_1}} - \rho_{p_2}\,(\mu - m)^{\frac{2}{4-p_2}}.$$

The function g is continuous in $[0,\mu]$, of class C^2 in $(0,\mu)$ and

$$g''(m) = -\frac{2(p_1-2)}{(4-p_1)^2}\,\rho_{p_1} m^{\frac{2(p_1-3)}{4-p_1}} - \frac{2(p_2-2)}{(4-p_2)^2}\,\rho_{p_2}(\mu-m)^{\frac{2(p_2-3)}{4-p_2}} < 0 \quad \forall\, m \in (0,\mu),$$

hence g attains the minimum either at 0 or at μ, entailing the thesis. □

In the next proposition, we give a more precise characterization of (3.9) when $p_1 \neq p_2$.

Proposition 3.3.1. Let $p_i \in (2,4)$ for $i = 1,2$, with $p_1 \neq p_2$. Then, given $\mu^\star$ as in (3.8), there results that

$$\mathcal{F}^\infty(\mu) = \begin{cases} \mathcal{E}_{p_1}(\mu) & \text{if} \quad (p_1 - p_2)(\mu - \mu^\star) > 0, \\ \mathcal{E}_{p_2}(\mu) & \text{if} \quad (p_1 - p_2)(\mu - \mu^\star) < 0. \end{cases}$$

Proof. Let us introduce for every $\mu > 0$ the function

$$h(\mu) := \mathcal{E}_{p_1}(\mu, \mathbb{R}^2) - \mathcal{E}_{p_2}(\mu, \mathbb{R}^2) = -\rho_{p_1}\mu^{\frac{2}{4-p_1}} + \rho_{p_2}\mu^{\frac{2}{4-p_2}},$$

and observe that

$$\lim_{\mu\to 0} h(\mu) = 0, \qquad \lim_{\mu\to+\infty} h(\mu) = \begin{cases} -\infty, & \text{if} \quad p_1 > p_2, \\ +\infty, & \text{if} \quad p_1 < p_2, \end{cases}$$

By direct computation,

$$h'(\mu) = -\frac{2\rho_{p_1}}{4-p_1}\mu^{\frac{p_1-2}{4-p_1}} + \frac{2\rho_{p_2}}{4-p_2}\mu^{\frac{p_2-2}{4-p_2}},$$

hence there exists $\widetilde{\mu} > 0$ such that $h'(\mu) < 0$ if and only if $(p_1 - p_2)(\mu - \widetilde{\mu}) < 0$. This entails that $h(\mu) < 0$ if and only if $(p_1 - p_2)(\mu - \mu^\star) > 0$, with $\mu^\star$ being the only value for which $h(\mu) = 0$: the thesis follows from the definition of h. □

3.3.3 Modified Gagliardo-Nirenberg inequalities

We recall now some Gagliardo-Nirenberg inequalities that will be useful in the following. Let us start from the classical Gagliardo-Nirenberg inequality on $\mathbb{R}^2$: for every $p > 2$ [26, Theorem 1.3.7] there exists K_p such that

$$\|u\|^p_{L^p(\mathbb{R}^2)} \leqslant K_p \|\nabla u\|^{p-2}_{L^2(\mathbb{R}^2)}\|u\|^2_{L^2(\mathbb{R}^2)} \qquad \forall u \in H^1(\mathbb{R}^2).$$

Let us now present some modified Gagliardo-Nirenberg inequalities proved in [3, 25] valid for functions in

$$\mathcal{D} = \{u \in L^2(\mathbb{R}^2) : \exists\, q \in \mathbb{C}, \lambda > 0 : u - q\mathcal{G}_\lambda := \phi_\lambda \in H^1(\mathbb{R}^2)\}.$$

First of all, let us observe that for $\sigma \in \mathbb{R}$ and $\lambda > 4e^{-4\pi\sigma-2\gamma}$ the space $\mathcal{D}$ can be equipped with the norm

$$\mathcal{N}_{\sigma,\lambda}(u) := (Q_\sigma(u) + \lambda\|u\|_2^2)^{\frac{1}{2}}. \tag{3.10}$$

The presence of such a limitation on the values of σ for the definition (3.10) is due to the fact that the quadratic form Q_σ is not positive and

$$\inf_{v\in\mathcal{D}\setminus\{0\}} \frac{Q_\sigma(v)}{\|v\|^2_{L^2(\mathbb{R}^2)}} = -4e^{-4\pi\sigma-2\gamma}.$$

On the one hand, the authors in [25] proved that there exists $C_p > 0$ such that

$$\|u\|^p_{L^p(\mathbb{R}^2)} \leqslant C_p\mathcal{N}_{\sigma,\lambda}(u)^{p-2}\|u\|^2_{L^2(\mathbb{R}^2)}, \qquad \forall\, u \in \mathcal{D}. \tag{3.11}$$

On the other hand, in [3] the authors proved the existence of a constant $M_p > 0$ such that every function $u = \phi_{\lambda(u)} + q\mathcal{G}_{\lambda(u)} \in \mathcal{D} \setminus H^1(\mathbb{R}^2)$, with $\lambda(u) = |q|^2/\|u\|_2^2$, satisfies

$$\|u\|^p_{L^p(\mathbb{R}^2)} \leqslant M_p(\left\|\nabla\phi_{\lambda(u)}\right\|^{p-2}_{L^2(\mathbb{R}^2)} + |q|^{p-2})\|u\|^2_{L^2(\mathbb{R}^2)}. \tag{3.12}$$

Let us observe that, differently from (3.11), in (3.12) the authors take advantage of a specific representation of the functions $u \in \mathcal{D} \setminus H^1(\mathbb{R}^2)$, in which the parameter λ depends on the function u itself.

3.4 Proof of the existence Theorem 3.2.1

This section is entirely devoted to the proof of Theorem 3.2.1 about the existence of ground states.

Proof of Theorem 3.2.1. Let $U_n = (u_{1,n}, u_{2,n})$ be a minimizing sequence for (3.4) at mass μ, i.e.

$$\|U_n\|_2^2 = \mu \quad \forall\, n \quad \text{and} \quad F(U_n) \to \mathcal{F}(\mu) \quad \text{as} \quad n \to +\infty,$$

and $q_{i,n}$ be the charge associated with $u_{i,n}$ for $i = 1, 2$. Let $\sigma = \min\{\sigma_1, \sigma_2\}$, fix $\lambda = 4e^{4\pi(2\beta-\sigma)-2\gamma}$ and consider the decomposition $u_{i,n} = \phi_{i,n} + q_{i,n}\mathcal{G}_\lambda$ for $i = 1, 2$: when not necessary, we omit the parameter λ to lighten the notation.

We divide the proof in three steps.
Step 1. There exist $\phi_i \in H^1(\mathbb{R}^2)$ and $q_i \in \mathbb{C}$ such that, up to subsequences,

$$\phi_{i,n} \rightharpoonup \phi_i \quad \textit{in} \quad H^1(\mathbb{R}^2), \quad q_{i,n} \to q_i \quad \textit{in} \quad \mathbb{C}.$$

By using that $\|U_n\|_2^2 = \mu$, (3.11) and (3.10) and observing that

$$(\sigma + \theta_\lambda)|q_{i,n}|^2 \leqslant (\sigma_i + \theta_\lambda)|q_{i,n}|^2 \leqslant \mathcal{N}_{\sigma_i}(u_{i,n})^2, \quad \forall\, n \in \mathbb{N}, \quad i = 1, 2,$$

one obtains that

$$\begin{aligned} F(U_n) \geqslant & \frac{1}{2}\mathcal{N}_{\sigma_1}(u_{1,n})^2 + \frac{1}{2}\mathcal{N}_{\sigma_2}(u_{2,n})^2 - \frac{\beta}{\sigma + \theta_\lambda}\mathcal{N}_{\sigma_1}(u_{1,n})\mathcal{N}_{\sigma_2}(u_{2,n}) \\ & - \frac{\lambda}{2}\mu - \frac{C_{p_1}\,\mu}{p_1}\mathcal{N}_{\sigma_1}(u_{1,n})^{p_1-2} - \frac{C_{p_2}\,\mu}{p_2}\mathcal{N}_{\sigma_2}(u_{2,n})^{p_2-2} \end{aligned} \tag{3.13}$$

Since $\sigma + \theta_\lambda = 2\beta$ according to our choice of λ, (3.13) entails

$$F(U_n) \geqslant \frac{1}{4}\mathcal{N}_{\sigma_1}(u_{1,n})^2 + \frac{1}{4}\mathcal{N}_{\sigma_2}(u_{2,n})^2 - \frac{C_{p_1}\,\mu}{p_1}\mathcal{N}_{\sigma_1}(u_{1,n})^{p_1-2} - \frac{C_{p_2}\,\mu}{p_2}\mathcal{N}_{\sigma_2}(u_{2,n})^{p_2-2} - \frac{\lambda}{2}\mu. \tag{3.14}$$

Since $F(U_n) < 0$ and $p_i < 4$, by (3.14) it follows that $\mathcal{N}_{\sigma_i}(u_{i,n})$ are equibounded for $i = 1, 2$, in particular $\phi_{i,n}$ are equibounded in $H^1(\mathbb{R}^2)$ and $q_{i,n}$ are equibounded in $\mathbb{C}$, hence by Banach-Alaoglu-Bourbaki theorem the thesis of Step 1 follows.

Step 2. It holds that $\mathcal{F}(\mu) < \mathcal{F}^\infty(\mu)$. By lemma 3.3.1 and [3, Proposition 3.2], we have that

$$\mathcal{F}^\infty(\mu) = \min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\} > \min\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\}. \tag{3.15}$$

Moreover, let us notice that

$$\inf_{U \in \Lambda_\mu} F(U) = \inf_{U \in \Lambda_\mu} \{F_1(u) + F_2(v) - \beta|q_1|\,|q_2|\} \quad \forall\, \mu > 0. \tag{3.16}$$

Indeed, on the one hand it holds for every $U = (u, v) \in \Lambda_\mu$ that $F(U) \geqslant F_1(u) + F_2(v) - \beta|q_1||q_2|$. On the other hand, if $u = \phi_1 + q_1\mathcal{G}_\lambda$ and $v = \phi_2 + q_2\mathcal{G}_\lambda$, then it is possible to find a proper phase factor $e^{i\theta}$ such that the function $\widetilde{U} = (u, e^{i\theta}v)$ satisfies

$$\mathrm{Re}\left\{q_1\overline{e^{i\theta}q_2}\right\} = |q_1||q_2|,$$

hence passing to the infimum the equality is achieved.
By (3.16), it follows that

$$\begin{aligned}\mathcal{F}(\mu) = \inf_{U\in\Lambda_\mu} F(U) &= \inf_{U\in\Lambda_\mu}\{F_1(u)+F_2(v)-\beta|q_1|\,|q_2|\}\\ &\leqslant \inf_{U\in\Lambda_\mu}\{F_1(u)+F_2(v)\}\\ &= \inf_{t\in[0,\mu]}\{\mathcal{F}_1(t)+\mathcal{F}_2(\mu-t)\}.\end{aligned} \tag{3.17}$$

Since $\mathcal{F}_1$ and $\mathcal{F}_2$ are strictly concave functions of the mass by [4, Lemma 4.2], then also the function $\mathcal{F}_1(t)+\mathcal{F}_2(\mu-t)$ turns out to be a strictly concave function of t and attains its minimum at $t=0$ or $t=\mu$, so that

$$\inf_{t\in[0,\mu]}\{\mathcal{F}_1(t)+\mathcal{F}_2(\mu-t)\} = \min\{\mathcal{F}_1(\mu),\mathcal{F}_2(\mu)\}. \tag{3.18}$$

By combining (3.15), (3.17) and (3.18), we conclude the proof of Step 2.

Step 3. The function $U=(u_1,u_2)=(\phi_1+q_1\mathcal{G}_\lambda,\phi_2+q_2\mathcal{G}_\lambda)$ is a ground state of (3.4) at mass μ. By Step 1, we deduce that $u_{i,n}\rightharpoonup u_i$ weakly in $L^2(\mathbb{R}^2)$ since $\phi_{i,n}\rightharpoonup\phi_i$ weakly in $L^2(\mathbb{R}^2)$ and $q_{i,n}\mathcal{G}_\lambda\to q_i\mathcal{G}_\lambda$ in $L^2(\mathbb{R}^2)$.

Set now $m=\|U\|^2_{L^2(\mathcal{I})}:=\|u_1\|^2_{L^2(\mathbb{R}^2)}+\|u_2\|^2_{L^2(\mathbb{R}^2)}$. First, we observe that by weak lower semicontinuity of the norms

$$\|u_1\|^2_{L^2(\mathbb{R}^2)}+\|u_2\|^2_{L^2(\mathbb{R}^2)}\leqslant\liminf_{n\to+\infty}\|u_{1,n}\|^2_{L^2(\mathbb{R}^2)}+\liminf_{n\to+\infty}\|u_{2,n}\|^2_{L^2(\mathbb{R}^2)}\leqslant\liminf_{n\to+\infty}\|U_n\|^2_{L^2(\mathcal{I})},$$

thus $m\leqslant\mu$.

Suppose first that $m=0$, i.e. $u\equiv0$ and $v\equiv0$. In particular, this entails that $q_{1,n}\to0$ and $q_{2,n}\to0$ as $n\to+\infty$. Therefore, relying on Step 2 we deduce that for n sufficiently large

$$\begin{aligned}\mathcal{F}^\infty(\mu)>\mathcal{F}(\mu)&=\lim_{n\to+\infty}\{F_1(u_{1,n})+F_2(u_{2,n})-\beta\,|q_{1,n}|\,|q_{2,n}|\}\\ &=\lim_{n\to+\infty}\{E_{p_1}(\phi_{1,n})+E_{p_2}(\phi_{2,n})\}\\ &\geqslant\lim_{n\to+\infty}\left\{\mathcal{E}_{p_1}(\|\phi_{1,n}\|_2^2)+\mathcal{E}_{p_2}(\|\phi_{2,n}\|_2^2)\right\}\\ &=\lim_{n\to+\infty}\left\{\mathcal{E}_{p_1}(\|u_{1,n}\|_2^2)+\mathcal{E}_{p_2}(\|u_{2,n}\|_2^2)\right\}\\ &\geqslant\inf\{\mathcal{E}_{p_1}(\mu_1)\,+\,\mathcal{E}_{p_2}(\mu_2):\mu_1+\mu_2=\mu\}=\mathcal{F}^\infty(\mu),\end{aligned}$$

thus $m\neq0$.

Suppose now that $0<m<\mu$. Note that, since $u_{i,n}\rightharpoonup u_i$ in $L^2(\mathbb{R}^2)$ for $i=1,2$, then

$$\|U_n-U\|^2_{L^2(\mathcal{I})}=\|U_n\|_2^2-\|U\|_2^2+o(1)=\mu-m+o(1),\quad\text{as}\quad n\to+\infty. \tag{3.19}$$

On the one hand, since $p_i>2$ for $i=1,2$, $\frac{\mu}{\|U_n-U\|_2^2}=\frac{\mu}{\mu-m}+o(1)>1$ as $n\to+\infty$ by

(3.19) and $\left\|\sqrt{\frac{\mu}{\|U_n-U\|_2^2}}(U_n-U)\right\|_2^2=\mu$, there results that

$$\begin{aligned}\mathcal{F}(\mu) &\leqslant F\left(\sqrt{\frac{\mu}{\|U_n-U\|_2^2}}(U_n-U)\right)\\ &= \frac{1}{2}\frac{\mu}{\|U_n-U\|_2^2}Q(U_n-U)-\sum_{i=1,2}\frac{1}{p_i}\left(\frac{\mu}{\|U_n-U\|_2^2}\right)^{\frac{p_i}{2}}\|u_{i,n}-u_i\|_{p_i}^{p_i}\\ &< \frac{\mu}{\|U_n-U\|_{L^2(\mathcal{I})}^2}F(U_n-U),\end{aligned}$$

hence

$$\liminf_{n\to+\infty}F(U_n-U)\geqslant\frac{\mu-m}{\mu}\mathcal{F}(\mu). \tag{3.20}$$

On the other hand, by similar computations

$$\mathcal{F}(\mu)\leqslant F\left(\sqrt{\frac{\mu}{\|U\|_2^2}}U\right)<\frac{\mu}{\|U\|_2^2}F(U)$$

thus

$$F(U)>\frac{m}{\mu}\mathcal{F}(\mu). \tag{3.21}$$

In addition, since $u_{i,n}\rightharpoonup u_i$ in $L^2(\mathbb{R}^2)$, $\phi_{i,n}\rightharpoonup\phi_i$ in $H^1(\mathbb{R}^2)$ and $q_{i,n}\to q_i$ in $\mathbb{C}$, then

$$Q(U_n-U)=Q(U_n)-Q(U)+o(1),\quad\text{as}\quad n\to+\infty,$$

while by Brezis-Lieb lemma [22] applied to $u_{i,n}$ we get

$$\|u_{i,n}\|_{L^{p_i}(\mathbb{R}^2)}^{p_i}=\|u_{i,n}-u\|_{L^{p_i}(\mathbb{R}^2)}^{p_i}+\|u\|_{L^{p_i}(\mathbb{R}^2)}^{p_i}+o(1),\quad\text{as}\quad n\to+\infty.$$

Thus

$$F(U_n)=F(U_n-U)+F(U)+o(1),\quad\text{as}\quad n\to+\infty. \tag{3.22}$$

Combining (3.20), (3.21) and (3.22), it follows that

$$\mathcal{F}(\mu)=\liminf_{n\to+\infty}F(U_n)=\liminf_{n\to+\infty}F(U_n-U)+F(U)>\frac{\mu-m}{\mu}\mathcal{F}(\mu)+\frac{m}{\mu}\mathcal{F}(\mu)=\mathcal{F}(\mu),$$

which, being a contradiction, forces $m=\mu$. In particular, $U\in\Lambda_\mu$ and thus $u_{i,n}\to u_i$ in $L^2(\mathbb{R}^2)$ and $\phi_{i,n}\to\phi_i$ in $L^2(\mathbb{R}^2)$.

In order to conclude that U is a ground state, we are left to prove that

$$F(U)\leqslant\liminf_{n\to+\infty}F(U_n)=\mathcal{F}(\mu),$$

which reduces to prove that $u_{i,n}\to u_i$ in $L^{p_i}(\mathbb{R}^2)$ for $i=1,2$. By (3.11), we obtain that

$$\|u_{i,n}-u_i\|_{L^{p_i}(\mathbb{R}^2)}^{p_i}\leqslant C_{p_i}\mathcal{N}_{\sigma_i}(u_{i,n}-u_i)^{p_i-2}\|u_{i,n}-u_i\|_{L^2(\mathbb{R}^2)}^2\to0,\quad\text{as}\quad n\to+\infty,$$

which concludes the proof since $\mathcal{N}_{\sigma_i}(u_{i,n}-u_i)$ is equibounded and $u_{i,n}\to u_i$ in $L^2(\mathbb{R}^2)$. □

Remark 3.4.1. Let us stress that the choice of λ in the proof of Theorem 3.2.1 is not the only possible one: it is sufficient to choose $\lambda>0$ such that $\sigma+\theta_\lambda>2\beta$ and all the arguments in the proof can be repeated.

3.5 Properties of ground states: proof of Theorem 3.2.2

This section is dedicated to the proof of the Theorem 3.2.2. The first result deals with the case $\beta > 0$ and establishes that $u_i \not\equiv 0$ and $q_i > 0$ for $i = 1, 2$, up to the multiplication by a phase factor.

Proposition 3.5.1. Let $p_i \in (2, 4)$, $\sigma_i \in \mathbb{R}$ for $i = 1, 2$, $\beta > 0$ and $\mu > 0$. Let $U = (u_1, u_2) \in \Lambda_\mu$ be a ground state of $\mathcal{F}$ at mass μ, then $u_i \not\equiv 0$ and $q_i > 0$ for $i = 1, 2$, up to a multiplication by a phase factor. Moreover, for $i = 1, 2$ and $\lambda_i > 0$ there results that $\phi_i := u_i - q_i \mathcal{G}_{\lambda_i} \not\equiv 0$.

Proof. Let $U = (u_1, u_2)$ be a ground state of F at mass μ and $\lambda_i > 0$ for $i = 1, 2$, so that $u_i = \phi_i + q_i \mathcal{G}_{\lambda_i}$. Since U solves (3.5), there results that

$$\begin{cases} \phi_1(0) &= (\sigma_1 + \theta_{\lambda_1}) q_1 - \beta\, q_2, \\ \phi_2(0) &= -\beta\, q_1 + (\sigma_2 + \theta_{\lambda_2}) q_2. \end{cases}$$

Step 1. $u_i \not\equiv 0$ for $i = 1, 2$. Let us first prove that $u_1 \not\equiv 0$. Suppose by contradiction that $u_1 \equiv 0$. Therefore, since $\beta > 0$, it follows that $q_2 = 0$, hence $u_2 \in H^1(\mathbb{R}^2)$. Therefore, since U is a ground state of F at mass μ, by Step 2 in Theorem 3.2.1 it holds that

$$\mathcal{F}(\mu) = F(U) = F_2(u_2) = \mathcal{E}_{p_2}(\mu) \geqslant \mathcal{F}^\infty(\mu) > \mathcal{F}(\mu),$$

which is a contradiction. Analogously, one can prove that $u_2 \not\equiv 0$.

Step 2. $q_i \neq 0$ for $i = 1, 2$. Let us first prove that $q_1 \neq 0$. If we suppose by contradiction that $q_1 = 0$, then

$$F(U) = E_{p_1}(u_1) + F_2(u_2) = \inf_{(u_1, u_2) \in \Lambda_\mu} \{E_{p_1}(u_1) + F_2(u_2)\}.$$

In particular, since the problems on the two planes are decoupled in this case, one can argue as in the proof of Lemma 3.3.1 and prove that

$$F(U) = \inf_{(u_1, u_2) \in \Lambda_\mu} \{E_{p_1}(u_1) + F_2(u_2)\} = \inf_{m \in [0, \mu]} \{\mathcal{E}_{p_1}(m) + \mathcal{F}_2(\mu - m)\}. \tag{3.23}$$

Since both $\mathcal{E}_{p_1}$ and $\mathcal{F}_2$ are strictly concave functions of the mass, then also the function $m \mapsto \mathcal{E}_{p_1}(m) + \mathcal{F}_2(\mu - m)$ is strictly concave in $[0, \mu]$ and attains its minimum at $m = 0$ or $m = \mu$. If one considers $U = (u_1, u_2)$ with $u_i \not\equiv 0$ for $i = 1, 2$, then U cannot realize the infimum in (3.23): indeed, if this is the case, then by strict concavity of the function $m \mapsto \mathcal{E}_{p_1}(m) + \mathcal{F}_2(\mu - m)$ there exists a function $\widetilde{U}$ with either $u_1 \equiv 0$ or $u_2 \equiv 0$ with energy strictly less than the energy of U, contradicting the hypothesis that U is a ground state of F. Therefore, it holds that either $u_1 \equiv 0$ or $u_2 \equiv 0$, but this is in contradiction with Step 1. In the same way, it is possible to prove that $q_2 \neq 0$, concluding the proof of Step 2.

Step 3. $\phi_i \not\equiv 0$ for $i = 1, 2$. Let us prove first that $\phi_1 \not\equiv 0$. Indeed, if we suppose by contradiction that $\phi_1 \equiv 0$, then by the first equation in (3.5) we have that

$$\omega - \lambda_1 = |q_1|^{p_1 - 2} \mathcal{G}_{\lambda_1}^{p_1 - 2}(x), \qquad \forall\, x \in \mathbb{R}^2 \setminus \{0\},$$

but this is a contradiction since the left-hand side is constant, while the right-hand side is a multiple of $\mathcal{G}_{\lambda_1}$, hence $\phi_1 \not\equiv 0$. Analogously, one can show that $\phi_2 \not\equiv 0$.

Step 4. $q_i > 0$ for $i = 1, 2$, up to a phase factor. First of all, let us observe that $q_1 = |q_1|e^{i\varphi_1}$ and $q_2 = |q_2|e^{i\varphi_2}$ share the same phase, i.e. $e^{i\varphi_1} = e^{i\varphi_2}$. Indeed, suppose by contradiction that $e^{i\varphi_1} \neq e^{i\varphi_2}$. Then the function $U_\varphi = (u_1, e^{i(\varphi_1-\varphi_2)}u_2)$ satisfies $\|U_\varphi\|_2^2 = \|U\|_2^2$ and

$$\begin{aligned} F(U_\varphi) &= F_1(u_1) + F_2\left(u_2 e^{i(\varphi_1-\varphi_2)}\right) - \beta \mathrm{Re}\{q_1\overline{q_2}e^{-i(\varphi_1-\varphi_2)}\} \\ &= F_1(u_1) + F_2(u_2) - \beta|q_1||q_2| \\ &< F_1(u_1) + F_2(u_2) - \beta \mathrm{Re}\{q_1\overline{q_2}\} = F(U), \end{aligned}$$

which contradicts the fact that U is a ground state of F at mass μ. Now, if q_i are not positive, i.e. $q_i = |q_i|e^{i\varphi}$ with $e^{i\varphi} \neq 1$, then it is sufficient to observe that the function $e^{-i\varphi}U$ has positive charges q_i and satisfies $\|e^{-i\varphi}U\|_2^2 = \mu$ and $F\left(e^{-i\varphi}U\right) = F(U)$, thus without loss of generality we can suppose that $q_i > 0$ for $i = 1, 2$. □

In order to prove Theorem 3.2.2, we follow the strategy introduced in [3] and [4], where the properties of ground states are proved switching to alternative minimization problems and relying on the connection between them and the original problem itself. In particular, we first introduce the action functional S_ω. Given $\omega \in \mathbb{R}$, the action functional at frequency ω is the functional $S_\omega : \Lambda \to \mathbb{R}$ defined by

$$S_\omega(U) = F(U) + \frac{\omega}{2}\|U\|_{L^2(\mathcal{I})}^2,$$

where $L^2(\mathcal{I}) := L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2)$. Denoted by $I_\omega : \Lambda \to \mathbb{R}$ the functional

$$I_\omega(U) = Q(U) + \omega\|U\|_{L^2(\mathcal{I})}^2 - \|u_1\|_{L^{p_1}(\mathbb{R}^2)}^{p_1} - \|u_2\|_{L^{p_2}(\mathbb{R}^2)}^{p_2}, \tag{3.24}$$

one defines the Nehari's manifold at frequency ω as

$$N_\omega := \{U \in \Lambda \setminus \{0\} : I_\omega(U) = 0\},$$

Let us also introduce

$$Q_\omega(U) := Q(U) + \omega\|U\|_{L^2(\mathcal{I})}^2.$$

Definition 3.5.2. A function U belonging to the Nehari manifold N_ω and satisfying

$$S_\omega(U) = d(\omega) := \inf_{V \in N_\omega} S_\omega(V)$$

is called a minimizer of the action at frequency ω.

Let us highlight that also minimizers of the action at frequency ω satisfy (3.2). In the next lemma, we state a connection between ground states at fixed mass and minimizers of the action at fixed frequency. The proof is analogous to the case of the standard NLS [29, 42]. Before stating it, let us define by

$$\omega^\star := -\inf_{U \in \Lambda\setminus\{0\}} \frac{Q(U)}{\|U\|_2^2}.$$

Lemma 3.5.1. *Let $\mu > 0$. If U is a ground state of F at mass μ, then U is a minimizer of the action at frequency*

$$\omega = \mu^{-1}\Big(\|u_1\|^{p_1}_{L^{p_1}(\mathbb{R}^2)} + \|u_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)} - Q(U)\Big) > \omega^\star. \tag{3.25}$$

Proof. Let $U = (u_1, u_2)$ be a ground state of F at mass μ and $\omega > 0$ be the associated Lagrange multiplier, given by (3.25). Assume by contradiction that there exists $V = (v_1, v_2) \in N_\omega$ such that $S_\omega(V) < S_\omega(U)$ and let $\tau > 0$ be such that $||\tau V||^2_{L^2(\mathbb{R}^2)} = \mu$. Then

$$S_\omega(\tau V) = \frac{\tau^2}{2} Q_\omega(V) - \frac{\tau^{p_1}}{p_1}\|v_1\|^{p_1}_{L^{p_1}(\mathbb{R}^2)} - \frac{\tau^{p_2}}{p_2}\|v_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)}.$$

Computing the derivative with respect to τ and using that $V \in N_\omega$, we get

$$\frac{d}{d\tau} S_\omega(\tau V) = \tau\left[(1-\tau^{p_1-2})\|v_1\|^{p_1}_{p_1} + (1-\tau^{p_2-2})\|v_2\|^{p_2}_{p_2}\right],$$

which is greater than equal to zero if and only if $0 < \tau \leqslant 1$. Hence $S_\omega(\tau V) \leqslant S_\omega(V) < S_\omega(U)$ for every $\tau > 0$ which, combined with $||\tau V||^2_2 = \|U\|^2_2 = \mu$, entails that $F(\tau V) < F(U)$. Since this contradicts the fact that U is a ground state of F at mass μ, it follows that U is a minimizer of the action at frequency ω.
Finally, (3.25) follows from

$$\begin{aligned} -\omega = \frac{Q(U) - \|u_1\|^{p_1}_{p_1} - \|u_2\|^{p_2}_{p_2}}{\mu} &= \frac{2F(U) - \frac{p_1-2}{p_1}\|u_1\|^{p_1}_{p_1} - \frac{p_2-2}{p_2}\|u_2\|^{p_2}_{p_2}}{\mu} \\ < 2\frac{\mathcal{F}(\mu)}{\mu} < \inf_{U\in\Lambda_\mu} \frac{Q(U)}{\mu} &= -\omega^\star. \end{aligned}$$

□

Let us now introduce the functionals $\widetilde{S}, A_\omega, B_\omega : \Lambda \to \mathbb{R}$, defined as

$$\begin{aligned} \widetilde{S}(U) &:= \frac{p_1-2}{2p_1}\|u_1\|^{p_1}_{L^{p_1}(\mathbb{R}^2)} + \frac{p_2-2}{2p_2}\|u_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)}, \\ A_\omega(U) &:= \frac{p_1-2}{2p_1} Q_\omega(U) + \frac{p_2-p_1}{p_1p_2}\|u_2\|^{p_2}_{L^{p_2}(\mathbb{R}^2)}, \\ B_\omega(U) &:= \frac{p_2-2}{2p_2} Q_\omega(U) + \frac{p_1-p_2}{p_1p_2}\|u_1\|^{p_1}_{L^{p_1}(\mathbb{R}^2)}, \end{aligned}$$

and observe that, by using (3.24), the action can be rewritten alternatively as

$$S_\omega(U) = \frac{1}{2} I_\omega(U) + \widetilde{S}(U) = \frac{1}{p_1} I_\omega(U) + A_\omega(U) = \frac{1}{p_2} I_\omega(U) + B_\omega(U),$$

so that

$$d(\omega) = \inf_{U\in N_\omega} \widetilde{S}(U) = \inf_{U\in N_\omega} A_\omega(U) = \inf_{U\in N_\omega} B_\omega(U).$$

In the following lemmas, we provide other equivalent formulations for $d(\omega)$ involving the three functionals $\widetilde{S}$, A_ω and B_ω subject to other constraints. For the proofs, we refer to [4, Lemma 5.6-5.7], where the same results were proved in an analogous setting.

Lemma 3.5.2. *Let $p_i > 2$ for $i = 1, 2$ and $\omega > \omega^\star$. Then, denoted with*

$$\widetilde{N}_\omega := \{V \in \Lambda \setminus \{0\},\, I_\omega(V) \leqslant 0\},$$

there results that

$$d(\omega) = \inf_{V \in \widetilde{N}_\omega} \widetilde{S}(V).$$

Moreover, for any function $U \in \Lambda \setminus \{0\}$, it holds that

$$\begin{cases} \widetilde{S}(U) = d(\omega) \\ I_\omega(U) \leqslant 0 \end{cases} \iff \begin{cases} S_\omega(U) = d(\omega) \\ I_\omega(U) = 0. \end{cases}$$

Lemma 3.5.3. *Let $p_i > 2$ for $i = 1, 2$ and $\omega > \omega^\star$. Then, denoted with*

$$\Pi_\omega := \{V \in \Lambda : \widetilde{S}(V) = d(\omega)\},$$

there results that

$$d(\omega) = \inf_{V \in \Pi_\omega} A_\omega(V) = \inf_{V \in \Pi_\omega} B_\omega(V).$$

In particular, for every $U \in \Lambda \setminus \{0\}$, it holds that

$$\begin{cases} A_\omega(U) = d(\omega) \\ U \in \Pi_\omega \end{cases} \iff \begin{cases} B_\omega(U) = d(\omega) \\ U \in \Pi_\omega \end{cases} \iff \begin{cases} S_\omega(U) = d(\omega) \\ I_\omega(U) = 0. \end{cases}$$

We are now ready to prove Theorem 3.2.2.

Proof of Theorem 3.2.2. Let us focus first on the proof of (3.6) and (3.7), when $\beta = 0$ and $\beta > 0$ respectively. In particular, if $\beta = 0$, then

$$\mathcal{F}(\mu) = \inf_{U \in \Lambda_\mu} \{F_1(u) + F_2(v)\} = \inf_{t \in [0,\mu]} \{\mathcal{F}_1(t) + \mathcal{F}_2(\mu - t)\},$$

hence by applying (3.18) we deduce (3.6) and the fact that every ground state is either of the form $U = (u_1, 0)$ or of the form $U = (0, u_2)$, depending on which is the minimum between $\mathcal{F}_1(\mu)$ and $\mathcal{F}_2(\mu)$: this entails in particular (i), (ii) and (iii) and the properties of the non-zero component.

If instead $\beta > 0$, then

$$\mathcal{F}(\mu) = \inf_{U \in \Lambda_\mu} \{F_1(u) + F_2(v) - \beta|q_1||q_2|\} \leqslant \inf_{t \in [0,\mu]} \{\mathcal{F}_1(t) + \mathcal{F}_2(\mu - t)\},$$

thus by (3.18) we get that

$$\mathcal{F}(\mu) \leqslant \min\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\}.$$

In order to prove (3.7), it is sufficient to exclude that $\mathcal{F}(\mu) = \min\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\}$. If we suppose by contradiction that $\mathcal{F}(\mu) = \min\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\}$, then there exist also ground states either of the form $U = (u_1, 0)$ or of the form $U = (0, u_2)$. But this contradicts Proposition 3.5.1, hence (3.7) holds.

Fix now $\beta > 0$ and let $U = (u_1, u_2)$ be a ground state of F at mass μ: its existence is ensured by Theorem 3.2.1. By proposition 3.5.1, we deduce that the associated charges q_i

satisfy $q_i > 0$ for $i = 1, 2$, up to multiplication by a phase factor. Moreover, by Lemma 3.5.1 U is also a minimizer of the action at frequency ω, with $\omega > \omega^\star$.

Let us now consider the decomposition of u_i corresponding to the Lagrange multiplier ω, namely $u_i = \phi_{i,\omega} + q_i \mathcal{G}_\omega$. Since the proof of the positivity and the radiality of $\phi_{i,\omega}$ and u_i is quite long, we divide it into three steps.

Step 1. Positivity of $\phi_{i,\omega}$ and u_i. We first prove that $\phi_{1,\omega} > 0$. Let us start defining the two sets

$$\Omega := \{x \in \mathbb{R}^2 \setminus \{0\} : \phi_{1,\omega}(x) \neq 0\}$$

and

$$\widehat{\Omega} := \{x \in \Omega : \alpha(x) \neq 0\},$$

where $\alpha : \Omega \to [0, 2\pi)$ is such that $\phi_{1,\omega}(x) = e^{i\alpha(x)}|\phi_{1,\omega}(x)|$. To prove that $\phi_{1,\omega} > 0$, we are reduced to prove that $\Omega = \mathbb{R}^2$ and $|\widehat{\Omega}| = 0$.

We start proving that $|\widehat{\Omega}| = 0$. Assume by contradiction that $\left|\widehat{\Omega}\right| > 0$ and introduce the function

$$U_\tau := (u_{1,\tau}, u_2), \quad \text{with} \quad u_{1,\tau} := \tau|\phi_{1,\omega}| + q_1 \mathcal{G}_\omega.$$

Let us observe that, since $\|\nabla|\phi_{1,\omega}|\|_2^2 \leqslant \|\nabla\phi_{1,\omega}\|_2^2$, then for every $\tau \in (-1, 1)$

$$\begin{aligned} Q_\omega(U_\tau) &= \tau^2 \left(\|\nabla|\phi_{1,\omega}|\|^2_{L^2(\mathbb{R}^2)} + \omega\|\phi_{1,\omega}\|_2^2\right) + |q_1|^2(\sigma_1 + \theta_\omega) + Q_{\sigma_2}(u_2) + \omega\|u_2\|_2^2 - \beta\, q_1\, q_2 \\ &< \|\nabla|\phi_{1,\omega}|\|^2_{L^2(\mathbb{R}^2)} + \omega\|\phi_{1,\omega}\|_2^2 + |q_1|^2(\sigma_1 + \theta_\omega) + Q_{\sigma_2}(u_2) + \omega\|u_2\|_2^2 - \beta\, q_1\, q_2 \\ &= Q_\omega(U_1) \leqslant Q_\omega(U). \end{aligned}$$

which entails in particular that

$$A_\omega(U_\tau) < A_\omega(U_1) \leqslant A_\omega(U) \quad \forall\, \tau \in (-1, 1).$$

We claim (and prove in Step 2) that there exists $\overline{\tau} \in (-1, 1)$ such that

$$\|u_{1,\overline{\tau}}\|_{p_1}^{p_1} = \|u_1\|_{p_1}^{p_1}. \tag{3.26}$$

In fact, if we prove (3.26), then $U_{\overline{\tau}} \in \Pi_\omega$ and $A_\omega(U_\tau) < A_\omega(U)$. On the other hand, U is a minimizer of A_ω on Π_ω by Lemma 3.5.3, but this generates a contradiction, ensuring that $|\widehat{\Omega}| = 0$ and $\phi_{1,\omega} > 0$ on Ω. Therefore, it is left to prove that $\Omega = \mathbb{R}^2$, i.e. $\phi_{1,\omega}(x) > 0$ for every $x \in \mathbb{R}^2$. First of all, $|\Omega| > 0$ by Proposition 3.5.1. Then, since u_1 solves (3.5), $\phi_{1,\omega}$ satisfies

$$(-\Delta + \omega)\phi_{1,\omega} = |u_1|^{p_1 - 2}(\phi_{1,\omega} + q_1 \mathcal{G}_\omega).$$

Therefore, as $\phi_{1,\omega}$ is non-negative, $(-\Delta + \omega)\phi_{1,\omega} \geqslant 0$ in $H^{-1}(\mathbb{R}^2)$ and $\phi_{1,\omega} \not\equiv 0$ by Proposition 3.5.1, then by the Strong Maximum Principle (e.g.,[26, Theorem 3.1.2]) $\phi_{1,\omega} > 0$ on $\mathbb{R}^2$. To prove that $\phi_{2,\omega}(x) > 0$ for every $x \in \mathbb{R}^2$, we repeat the same arguments using the functional B_ω instead of A_ω. The positivity of u_i follows from the positivity of $\phi_{i,\omega}$ and q_i.

Step 2. Proof of the claim (3.26). First of all, let us observe that the function $\tau \mapsto \|u_{1,\tau}\|_{p_1}^{p_1}$ is continuous on $[-1,1]$. Moreover, since

$$|u_1(x)|^2 = |\phi_{1,\omega}(x)|^2 + q_1^2\mathcal{G}_\omega^2(x) + 2\cos(\alpha)q_1|\phi_{1,\omega}(x)|\mathcal{G}_\omega(x) < |u_{1,1}(x)|^2, \quad \forall x \in \widehat{\Omega},$$

and $\left|\widehat{\Omega}\right| > 0$, there results that $\|u_1\|_{p_1}^{p_1} < \|u_{1,1}\|_{p_1}^{p_1}$. In order to prove (3.26), we need to distinguish two cases. Suppose first that there exists $\widetilde{\Omega}$, with $\left|\widetilde{\Omega}\right| > 0$, such that $\alpha \neq \pi$ on $\widetilde{\Omega}$. In this case, we have that

$$\begin{aligned}
\|u_{1,-1}\|_{L^{p_1}(\mathbb{R}^2)}^{p_1} &= \|u_{1,-1}\|_{L^{p_1}(\mathbb{R}^2\setminus\widetilde{\Omega})}^{p_1} + \|u_{1,-1}\|_{L^{p_1}(\widetilde{\Omega})}^{p_1} \\
&= \|u_1\|_{L^{p_1}(\mathbb{R}^2\setminus\widetilde{\Omega})}^{p_1} + \int_{\widetilde{\Omega}} \left||\phi_{1,\omega}|^2 + q_1^2\mathcal{G}_\omega^2 - 2\,q_1|\phi_{1,\omega}|\mathcal{G}_\omega\right|^{\frac{p_1}{2}} dx \\
&< \|u_1\|_{L^{p_1}(\mathbb{R}^2\setminus\widetilde{\Omega})}^{p_1} + \int_{\widetilde{\Omega}} \left||\phi_{1,\omega}|^2 + q_1^2\mathcal{G}_\omega^2 + 2\cos(\alpha)q_1|\phi_{1,\omega}|\mathcal{G}_\omega\right|^{\frac{p_1}{2}} dx \\
&= \|u_1\|_{L^{p_1}(\mathbb{R}^2)}^{p_1}
\end{aligned}$$

hence, since $\|u_{1,-1}\|_{L^{p_1}(\mathbb{R}^2)}^{p_1} < \|u_1\|_{L^{p_1}(\mathbb{R}^2)}^{p_1} < \|u_{1,1}\|_{L^{p_1}(\mathbb{R}^2)}^{p_1}$, there exists $\overline{\tau} \in (-1,1)$ such that (3.26) holds.

Suppose instead that $\alpha(x) = \pi$ for a.e. $x \in \Omega$: this choice of α can be reformulated also as $u_1(x) = u_{1,-1}(x)$ for a.e. $x \in \Omega$ or as $\phi_{1,\omega} = -|\phi_{1,\omega}|$ for a.e. $x \in \Omega$. Differently from the previous case, we cannot conclude immediately using the continuity of $\|u_{1,\tau}\|_{p_1}^{p_1}$ since $\|u_{1,-1}\|_{p_1}^{p_1} = \|u_1\|_{p_1}^{p_1}$. To solve this issue, we observe that for every $\tau \in [-1,1]$

$$\begin{aligned}
\left|\frac{d}{d\tau}|u_{1,\tau}|^{p_1}\right| &= \left|\frac{d}{d\tau}(\tau^2|\phi_{1,\omega}|^2 + q_1^2\mathcal{G}_\omega^2 + 2\tau q_1|\phi_{1,\omega}|\mathcal{G}_\omega)^{\frac{p_1}{2}}\right| \\
&= \left|p_1\,|\phi_{1,\omega}|\,|u_{1,\tau}|^{p_1-2}\,u_{1,\tau}\right| = p_1\,|\phi_{1,\omega}|\,|u_{1,\tau}|^{p_1-1} \leqslant p_1|\phi_{1,\omega}||u_{1,1}|^{p_1-1} \in L^1(\mathbb{R}^2),
\end{aligned}$$

hence by dominated convergence

$$\begin{aligned}
\frac{d}{d\tau}\|u_{1,\tau}\|_{L^{p_1}(\mathbb{R}^2)}^{p_1}\Big|_{\tau=-1^+} = \int_{\mathbb{R}^2} \frac{d}{d\tau}|u_{1,\tau}|^{p_1}\Big|_{\tau=-1} dx &= \int_{\mathbb{R}^2} p_1|\phi_{1,\omega}||u_{1,-1}|^{p_1-2}u_{1,-1}\,dx \\
&= \int_{\mathbb{R}^2} p_1|\phi_{1,\omega}||u_1|^{p_1-2}u_1\,dx.
\end{aligned}$$

Since U is a ground state and solves (3.5) with $\lambda_1 = \omega$, there results that

$$\langle \nabla\chi, \nabla\phi_{1,\omega}\rangle_{L^2(\mathbb{R}^2)} + \langle \chi, \omega\phi_{1,\omega} - |v|^{r-2}v\rangle_{L^2(\mathbb{R}^2)} = 0 \quad \forall\,\chi \in H^1(\mathbb{R}^2). \tag{3.27}$$

By choosing $\chi = |\phi_{1,\omega}|$ in (3.27) and recalling that $\phi_{1,\omega} = -|\phi_{1,\omega}|$ on Ω (and consequently in $\mathbb{R}^2$), it follows that

$$\int_{\mathbb{R}^2} |\phi_{1,\omega}(x)||u_1(x)|^{p_1-2}u_1(x)\,dx = -\int_{\mathbb{R}^2} |\nabla|\phi_{1,\omega}(x)||^2\,dx - \omega\int_{\mathbb{R}^2} |\phi_{1,\omega}(x)|^2\,dx,$$

thus

$$\frac{d}{d\tau}\|u_{1,\tau}\|_{L^{p_1}(\mathbb{R}^2)}^{p_1}\Big|_{\tau=-1^+} < 0. \tag{3.28}$$

Therefore, by combining (3.28) and the fact that $\|u_{1,-1}\|^{p_1}_{L^{p_1}(\mathbb{R}^2)} = \|u_1\|^{p_1}_{L^{p_1}(\mathbb{R}^2)} < \|u_{1,1}\|^{p_1}_{L^{p_1}(\mathbb{R}^2)}$, (3.26) follows.

Step 3. Radiality of $\phi_{i,\omega}$ and u_i. As done in Step 1, we recall that by lemma 3.5.3 U is also a minimizer of A_ω in Π_ω. In order to prove that $\phi_{1,\omega}$ and u_1 are radially symmetric and decreasing along the radial direction, it is sufficient to show that $\phi_{1,\omega} = \phi^\star_{1,\omega}$ a.e. on $\mathbb{R}^2$, where $\phi^\star_{1,\omega}$ denotes the symmetric decreasing rearrangement of $\phi_{1,\omega}$.

For the sake of completeness, let us recall that, given a nonnegative function $f \in L^p(\mathbb{R}^n)$, the symmetric decreasing rearrangement f^* is defined as

$$f^\star(x) := \int_0^{+\infty} \mathbb{1}_{B_{r(t)}}(x)\, dt, \quad r(t) := \sqrt{\frac{|\{x \,:\, f(x) > t\}|}{\pi}}.$$

Then the following relations hold for $\phi^\star_{1,\omega}$ (see for example [3, Section 2.3]):

$$\|\nabla \phi^\star_{1,\omega}\|_2^2 \leqslant \|\nabla \phi_{1,\omega}\|_2^2, \qquad \|\phi^\star_{1,\omega}\|_2^2 = \|\phi_{1,\omega}\|_2^2, \tag{3.29}$$

$$\forall\, p > 1 \quad \forall\, g \in L^p(\mathbb{R}^2) \quad \|\phi^\star_{1,\omega} + g^\star\|_p^p \geqslant \|\phi_{1,\omega} + g\|_p^p. \tag{3.30}$$

Moreover, if g is radially symmetric and decreasing, then the equality in (3.30) holds if and only if $\phi^\star_{1,\omega} = \phi_{1,\omega}$ a.e. on $\mathbb{R}^2$ (see again [3, Section 2.3]).

Assume now by contradiction that $\phi_{1,\omega} \neq \phi^\star_{1,\omega}$ on a set of non-zero Lebesgue measure, and define the function $U^\star := (\phi^\star_{1,\omega} + q_1 \mathcal{G}_\omega, u_2)$. By (3.29) and the fact that the equality case in (3.30) is realized if and only if $\phi^\star_{1,\omega} = \phi_{1,\omega}$ a.e. on $\mathbb{R}^2$, we get that $A_\omega(U^\star) \leqslant A_\omega(U)$ and $\|\phi^\star_{1,\omega} + q_1\mathcal{G}_\omega\|^{p_1}_{p_1} > \|\phi_{1,\omega} + q_1\mathcal{G}_\omega\|^{p_1}_{p_1}$. In particular, there exists $\tau \in (0,1)$ such that, denoted with $U^\star_\tau = (\tau\phi^\star_{1,\omega} + q_1\mathcal{G}_\omega, u_2)$, there results that $\|\tau\phi^\star_{1,\omega} + q_1\mathcal{G}_\omega\|^{p_1}_{p_1} = \|\phi_{1,\omega} + q_1\mathcal{G}_\omega\|^{p_1}_{p_1}$, i.e. $U^\star_\tau \in \Pi_\omega$. Moreover, it holds that

$$\frac{p_1 - 2}{2p_1} Q_\omega(U^\star_\tau) - \frac{p_1 - 2}{2p_1} Q_\omega(U^\star) = -\frac{p_1 - 2}{2p_1}(1 - \tau^2)\left(\left\|\nabla \phi^\star_{1,\omega}\right\|_2^2 + \omega \left\|\phi^\star_{1,\omega}\right\|_2^2\right) < 0,$$

thus $A_\omega(U^\star_\tau) < A_\omega(U^\star) \leqslant A_\omega(U)$, which contradicts the fact that U is a minimizer of the action at frequency ω, hence $\phi_{1,\omega}$ and u_1 are radially symmetric and decreasing. The same properties can be proved for $\phi_{2,\omega}$ and u_2 (using the functional B_ω instead of A_ω), hence the proof is concluded. □

3.6 Proof of Theorems 3.2.4 and 3.2.5

This section is devoted to the proof of Theorem 3.2.4 and Theorem 3.2.5. Let us start with the proof of Theorem 3.2.4.

Proof of the Theorem 3.2.4. Let us start with the proof of point (i). Let $U = (u_1, u_2)$ be a ground state of (3.4) at mass μ, q_i and μ_i be the charge and the mass associated with u_i for $i = 1, 2$. By Theorem 3.2.2, we can assume that q_i and u_i are positive for $i = 1, 2$. Suppose now by contradiction that $q_1 \leqslant q_2$ and consider the function $\widetilde{U} = (u_2, u_1) \in \Lambda_\mu$,

which satisfies

$$\begin{aligned} F(\widetilde{U}) &= F_1(u_2) + F_2(u_1) - \beta\, q_1\, q_2 \\ &= F_1(u_1) + \frac{\sigma_1}{2}\left(q_2^2 - q_1^2\right) + F_2(u_2) + \frac{\sigma_2}{2}\left(q_1^2 - q_2^2\right) - \beta q_1 q_2 \\ &= F_1(u_1) + F_2(u_2) - \beta q_1\, q_2 + \frac{(\sigma_2 - \sigma_1)}{2}(q_1^2 - q_2^2) \\ &= F(U) + \frac{(\sigma_2 - \sigma_1)}{2}(q_1^2 - q_2^2). \end{aligned} \tag{3.31}$$

In particular, if $q_1 < q_2$, then by (3.31) we get that $F(\widetilde{U}) < F(U)$, which contradicts the fact that U is a ground state. If instead $q_1 = q_2 =: q$, then $F(U) = F(\widetilde{U})$, hence $\widetilde{U}$ is a ground state too and solves (3.5). In particular, since both U and $\widetilde{U}$ solve (3.5), there results that

$$\begin{cases} \phi_{1,\omega}(0) = (\sigma_1 + \theta_\omega - \beta)q \\ \phi_{2,\omega}(0) = (\sigma_2 + \theta_\omega - \beta)q, \end{cases} \quad \text{and} \quad \begin{cases} \phi_{2,\omega}(0) = (\sigma_1 + \theta_\omega - \beta)q \\ \phi_{1,\omega}(0) = (\sigma_2 + \theta_\omega - \beta)q, \end{cases}$$

hence $\sigma_1 = \sigma_2$, which is again a contradiction and concludes the proof of point (1).

Let us focus now on the proof of point (ii). Fix $\beta > 0$, $\sigma_1 \in \mathbb{R}$, denote with $p := p_1 = p_2$ and let σ_2 vary in the interval $(\sigma_1, +\infty)$: let us denote with $\delta := \sigma_2 - \sigma_1 \in (0, +\infty)$. We observe that, by Theorem 3.2.1, there exists at least a ground state of (3.4) at mass μ, that we denote by $U_\delta = (u_{1,\delta}, u_{2,\delta})$. We consider for $i = 1, 2$ the decomposition $u_{i,\delta} = \phi_{i,\delta} + q_{i,\delta}\mathcal{G}_\lambda$, corresponding to $\lambda = 4e^{4\pi(2\beta - \sigma_1) - 2\gamma}$ or, equivalently, to $\sigma_1 + \theta_\lambda = 2\beta$, and we call m_δ the mass of $u_{1,\delta}$. By arguing as in (3.13) and using that $F(U_\delta) < 0$, we get that

$$\sum_{i=1,2}\left\{\frac{1}{4}\mathcal{N}_{\sigma_i}(u_{i,\delta})^2 - \frac{C_p\mu}{p}\mathcal{N}_{\sigma_i}(u_{i,\delta})^{p-2}\right\} < \frac{\lambda}{2}\mu,$$

thus $\mathcal{N}_{\sigma_i}(u_{i,\delta})$ are equibounded in $\delta > 0$ for $i = 1, 2$. In particular, this entails that $(\phi_{i,\delta})_{\delta>0}$ is equibounded in $H^1(\mathbb{R}^2)$ and both $(u_{i,\delta})_{\delta>0}$ and $(\phi_{i,\delta})_{\delta>0}$ are equibounded in $L^r(\mathbb{R}^2)$ for every $r \geqslant 2$ for $i = 1, 2$. Moreover, $(q_{1,\delta})_{\delta>0}$ is equibounded and

$$(\sigma_2 + \theta_\lambda)q_{2,\delta}^2 = (2\beta + \delta)q_{2,\delta}^2 \leqslant C,$$

from which we deduce that $q_{2,\delta} \to 0$ as $\delta \to +\infty$. Since by Lagrange theorem it holds that for every $r \geqslant 2$

$$|\|u_{2,\delta}\|_r^r - \|\phi_{2,\delta}\|_r^r| \leqslant r \sup\left\{\|u_{2,\delta}\|_r^{r-1}, \|\phi_{2,\delta}\|_r^{r-1}\right\}|q_{2,\delta}|\|\mathcal{G}_\lambda\|_r \to 0, \quad \delta \to +\infty,$$

it follows that

$$\begin{aligned} 0 > F_2(u_{2,\delta}) - E_p(\phi_{2,\delta}) =& \frac{\lambda}{2}\left(\|\phi_{2,\delta}\|_2^2 - \|u_{2,\delta}\|_2^2\right) + \frac{q_{2,\delta}^2}{2}(\sigma_1 + \delta + \theta_\lambda) \\ &- \frac{1}{p}\left(\|u_{2,\delta}\|_p^p - \|\phi_{2,\delta}\|_p^p\right) = \frac{\delta}{2}q_{2,\delta}^2 + o(1), \end{aligned}$$

hence $\delta q_{2,\delta}^2 \to 0$ as $\delta \to +\infty$. Therefore,

$$\begin{aligned}\mathcal{F}(\mu) = F(U_\delta) = F_1(u_{1,\delta}) + F_2(u_{2,\delta}) + o(1) &= F_1(u_{1,\delta}) + E_p(\phi_{2,\delta}) + o(1) \\ &\geqslant \mathcal{F}_1(m_\delta) + \mathcal{E}_p(\mu - m_\delta) + o(1), \quad \delta \to +\infty.\end{aligned} \tag{3.32}$$

On the other hand, since $\mathcal{F}_{\sigma,p}$ is an increasing function of σ by [4, Lemma 4.3] and (3.6)-(3.7) hold, we get that

$$\mathcal{F}(\mu) = F(U_\delta) \leqslant \min\{\mathcal{F}_1(\mu), \mathcal{F}_2(\mu)\} = \mathcal{F}_1(\mu),$$

thus combining with (3.32), there results that

$$\mathcal{F}_1(\mu) \geqslant \mathcal{F}_1(m_\delta) + \mathcal{E}_p(\mu - m_\delta) + o(1), \quad \delta \to +\infty. \tag{3.33}$$

We claim that $m_\delta \to \mu$ and $\mathcal{F}(\mu) \to \mathcal{F}_1(\mu)$. Indeed, if we suppose by contradiction that there exists $\delta_n \to +\infty$ as $n \to +\infty$ and $\varepsilon > 0$ such that $m_{\delta_n} \leqslant \mu - \varepsilon$ for every $n \in \mathbb{N}$, then by concavity of both $\mathcal{F}_1$ and $\mathcal{E}_p$ and since $\mathcal{F}_1(\mu) < \mathcal{E}_p(\mu)$ for every $\mu > 0$, we have that

$$\begin{aligned}\lim_{n\to+\infty}[\mathcal{F}_1(m_{\delta_n}) + \mathcal{E}_p(\mu - m_{\delta_n}) + o(1)] &\geqslant \inf_{m\in[0,\mu-\varepsilon]}\{\mathcal{F}_1(m) + \mathcal{E}_p(\mu - m)\} \\ &= \min\{\mathcal{E}_p(\mu), \mathcal{F}_1(\mu - \varepsilon) + \mathcal{E}_p(\varepsilon)\} \\ &> \min\{\mathcal{E}_p(\mu), \mathcal{F}_1(\mu)\} = \mathcal{F}_1(\mu),\end{aligned}$$

which is in contradiction with (3.33) and entails that $m_\delta \to \mu$ as $\delta \to +\infty$. Moreover, by (3.32) and (3.33), we deduce that $\mathcal{F}(\mu) \to \mathcal{F}_1(\mu)$, concluding the proof of point (ii).

□

We are now ready to prove Theorem 3.2.5.

Proof of Theorem 3.2.5. Given $\sigma = \sigma_1 = \sigma_2$, we know by Theorem 3.2.1 that there exists at least a ground state of (3.4) at mass μ, that we denote by $U_\sigma = (u_{1,\sigma}, u_{2,\sigma})$. Fixing $\lambda = 4e^{-2\gamma}$, we represent $u_{i,\sigma}$ as $u_{i,\sigma} = \phi_{i,\sigma} + q_{i,\sigma}\mathcal{G}_\lambda$ for $i = 1, 2$. By using (3.11) and the fact that $F(U_\sigma) < 0$, we get that for σ sufficiently large (3.14) holds, hence $\mathcal{N}_\sigma(u_{i,\sigma})$ is equibounded in $\sigma > 0$. This entails that $\sigma q_{i,\sigma}^2$ is bounded, hence $q_{i,\sigma} \to 0$ as $\sigma \to +\infty$ for $i = 1, 2$.

Therefore, as $\sigma \to +\infty$

$$\begin{aligned}\mathcal{F}(\mu) = F(U_\sigma) &= \sum_{i=1,2}\left\{\frac{1}{2}\|\nabla\phi_{i,\sigma}\|_2^2 + \frac{1}{2}\lambda\left(\|\phi_{i,\sigma}\|_2^2 - \|u_{i,\sigma}\|_2^2\right) - \frac{1}{p_i}\|u_{i,\sigma}\|_{p_i}^{p_i}\right\} + o(1) \\ &= \sum_{i=1,2} E_{p_i}(\phi_{i,\sigma}) + o(1) \geqslant \sum_{i=1,2}\mathcal{E}_{p_i}(\|\phi_{i,\sigma}\|_2^2) + o(1) \\ &= \sum_{i=1,2}\mathcal{E}_{p_i}(\|u_{i,\sigma}\|_2^2) + o(1) \geqslant \inf_{m\in[0,\mu]}\{\mathcal{E}_{p_1}(m) + \mathcal{E}_{p_2}(\mu - m)\} + o(1) \\ &= \min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\} + o(1).\end{aligned} \tag{3.34}$$

On the other hand, by Lemma 3.3.1 and Step 2 in the proof of Theorem 3.2.1, we have that $F(U_\sigma) = \mathcal{F}(\mu) < \mathcal{F}^\infty(\mu) = \min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\}$, thus together with (3.34) gives

$$\lim_{\sigma\to+\infty} F(U_\sigma) = \min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\}.$$

Let us distinguish now the cases $\mu < \mu^\star$ and $\mu > \mu^\star$. If $\mu < \mu^\star$, then by Proposition 3.3.1 there results that $\min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\} = \mathcal{E}_{p_1}(\mu)$ and

$$\lim_{\sigma\to+\infty} F(U_\sigma) = \mathcal{E}_{p_1}(\mu), \tag{3.35}$$

(3.35) entails also that $\|u_{1,\sigma}\|_2^2 \to \mu$ as $\sigma \to +\infty$. Indeed, if we suppose by contradiction that there exists $\varepsilon > 0$ such that $\|u_{1,\sigma}\|_2^2 \leqslant \mu - \varepsilon$ along a subsequence of $\sigma \to +\infty$, then arguing as in (3.34) we get that

$$\lim_{\sigma\to+\infty} F(U_\sigma) \geqslant \lim_{\sigma\to+\infty} \sum_{i=1,2} \mathcal{E}_{p_i}(\|u_{i,\sigma}\|_2^2) \geqslant \min\{\mathcal{E}_{p_1}(\mu-\varepsilon), \mathcal{E}_{p_2}(\mu)\} > \mathcal{E}_{p_1}(\mu),$$

which contradicts (3.35).

If instead $\mu > \mu^\star$, then $\min\{\mathcal{E}_{p_1}(\mu), \mathcal{E}_{p_2}(\mu)\} = \mathcal{E}_{p_2}(\mu)$, hence it is possible to deduce that $F(U_\sigma) \to \mathcal{E}_{p_2}(\mu)$ and $\|u_{2,\sigma}\|_2^2 \to \mu$ as done for the case $\mu < \mu^\star$, concluding the proof. □

Part II

Chapter 4

Qubit conversation in the photosynthesis process

Biological processes reveal abilities that are very impressive and cannot be adequately explained with the only use of traditional (classical) approaches. The biological system, from a mathematical and physical point of view, exhibits certain features [86] that must be included in the models that are intended to be constructed and which can make their treatment both challenging and fascinating at the same time. These systems are *open systems*: There is always an interaction between a subsystem and another, called the environment, usually characterized by a higher number of degrees of freedom. The biological system are *multi-component*: in the direction of possible models based on quantum mechanics, it is impossible not to consider various types of agents (as for example molecules with different structural and functional rules) interacting with each other. Finally, biological subsystems are strongly interacting and the role of quantum features as decoherence it must be adequately taken into account.
In a paper [84], quantum mechanics is involved in the mathematical model for the photosynthesis process in some marine algae at room temperature. The focus of this model is on how energy travels across the light-harvesting molecules involved in photosynthesis, showing in an experiment that quantum processes at physiological temperature are able to transfer energy almost without loss.
A certain amount of quantum mechanics is thought to be used by nature in order to enhance the efficiency of the underlying processes. The first question which arises then is: *How can quantum features survive in an open quantum system subject to permanent environmental noise*? A second question closely related to the experiments is: *Is it feasible to incorporate the interaction with the environment into the model in a manner that elucidates the enhancement of the efficiency of the transfer rate?*

In this chapter, we shall present a mathematical model for the illustration of the excitation energy transfer in photosynthesis complexes, with the aim of studying the "constructive" interplay between the coherent quantum excitation transfer and the vibrational classical motion of the underlying molecular structure. The model is based on

the Schrödinger equation associated with a time-dependent Hamiltonian, describing the propagation of an absorbed photon through a spin chain towards the reaction center of the photosynthesis apparatus (Spin-Boson model).

4.1 Applications of the Spin-Boson model

Before proceeding further, it's important to note that the effective transfer of (quantum) excitation or energy plays a crucial role across several domains, including molecular technology, quantum biology, and quantum heat engines. The Spin-Boson model, which we will present in subsection 4.2.1, serves as the foundational mathematical framework for characterizing these transfer processes. To appreciate its breadth of application, let us briefly discuss the three principal areas it impacts.

Excitation energy transfer in the photosynthesis process [53]:
Photosynthesis ranks as a crucial biological process on our planet, serving as the foundation of life by harnessing the plentiful energy from the sun and converting it into chemical energy. Specifically, chlorophyll-bearing entities such as plants, algae, and cyanobacteria capture a wide range of solar energy through their leaves. They channel the absorbed photons (through excitation transfer via a pigment network) to a reaction center, where these photons facilitate the photosynthesis process, specifically

$$6\,CO_2 + 6\,H_2O \rightarrow^{photons} 6\,O_2 + C_6H_{12}O_6\,, \qquad \Delta G = 2.87 * 10^3\ kJ/mol\,.$$

The sun's energy is thus transformed into a chemical energy, stored in the carbohydrate molecule, necessary for the growth of the plant (see Fig 4.1).

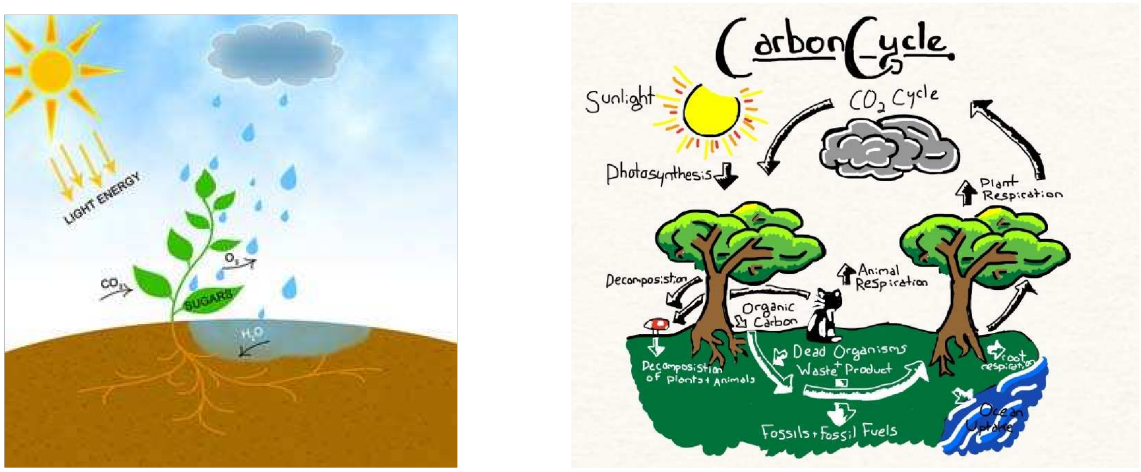


Figure 4.1: The photosynthesis process in plants on the left [https://study.com] and the carbon cycle on the right [https://quizizz.com].

Biological systems exhibit significant complexity, especially in the photosynthesis process, which comprises numerous distinct stages. Initially, the light reactions harness light

energy to produce energy-storage molecules. Subsequently, during the second stage, light-independent reactions utilize these molecules to capture and convert carbon dioxide.

In this model, our focus is solely on modeling and comprehending the efficient transfer of excitation energy, beginning with photon absorption and concluding with their arrival at the reaction center. The efficiency of this energy transfer in plants is notable; the likelihood that an absorbed photon aids in charge separation at the reaction center approaches nearly 100%. This mathematical problem shares profound similarities with the challenges encountered in quantum information.

Signal transfer in neural networks [60]:
Various biological processes appear to harness environmental noise to improve the efficiency of excitation transfer. Interestingly, certain behaviors in brain activity defy clear explanations within the framework of conventional neuroscience. For instance, existing biological memory models fail to account for the apparent synchronized firing of distant neurons. Moreover, traditional theories struggle to clarify the remarkable speed at which our brain processes information. Conceptualizing the brain as a quantum system might provide better insights into these challenges.

Neurons, which are cells in the nervous system, form the fundamental working unit of the brain. Each neuron comprises a cell body (soma), dendrites, extensions that can receive electrochemical signals from nearby neurons, and an axon that sends signals across synapses to other neurons (see Fig. 4.2). The human brain contains approximately 10^{11} nerve cells, organized into a dense network designed for receiving and transmitting information to other neurons. A distinctive feature of nerve cells is their ability to communicate with remarkable precision, despite being spaced apart. The essential components of a neuronal network include the processing element (neuron), the structures connecting neurons, network dynamics, and the learning rules that regulate changes in connection strengths. A basic depiction of a neuron involves a binary system with two distinct states: the ground state, where the neuron remains inactive, and the excited state, where the neuron is activated. Each neuron acts as a switch, with its synaptic connections to neighboring neurons being adjusted based on previous experiences, which constitutes learning.

In Section 4.2.1, we discussed the Spin-Boson model, which serves as a framework for illustrating the firing of neurons within a simplified neural network and the resulting decoherence caused by environmental interactions. The non-locality (or correlations between molecules that are not in close proximity) seen in the energy transfer during photosynthesis might be a key feature that explains the remarkable speed of information processing in the brain.

Information transfer via spin chains [63]:
Traditional communication occurs via mediums like radio channels, optical fibers, or copper wires, which convey the data unit (classical bit) through electromagnetic waves or optical pulses. However, at extremely small (quantum) scales, a novel approach is necessary to effectively transmit the quantum bit.

Effective communication among a quantum computer's various components, such as

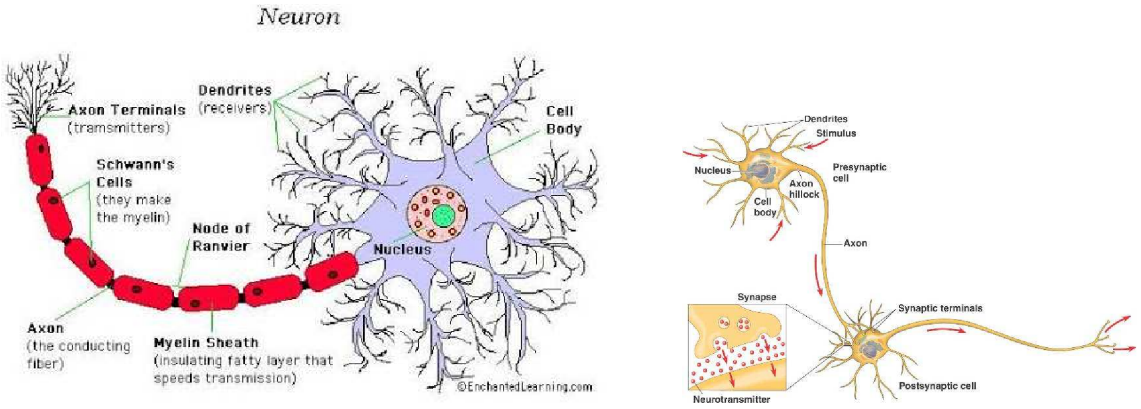


Figure 4.2: The axon (https://www.enchantedlearning.com) and the signal transfer through the nervous system (https://socratic.org)

quantum processors and memories, is crucial for its operation. This communication is vital not only for transferring information between locations, but also for creating entangled states between particles that are spatially apart a unique feature of quantum computers [52]. To address this need for communication, the concept of "quantum channel" has arisen. Spin chains represent a promising group of systems that can act as dependable quantum channels. These chains consist of interacting two-level systems (spins) organized on a graph (refer to Fig. 4.3), with their behavior dictated by an appropriate Hamiltonian. The Spin-Boson model, which we will introduce in the following section, is fundamental to this subject.

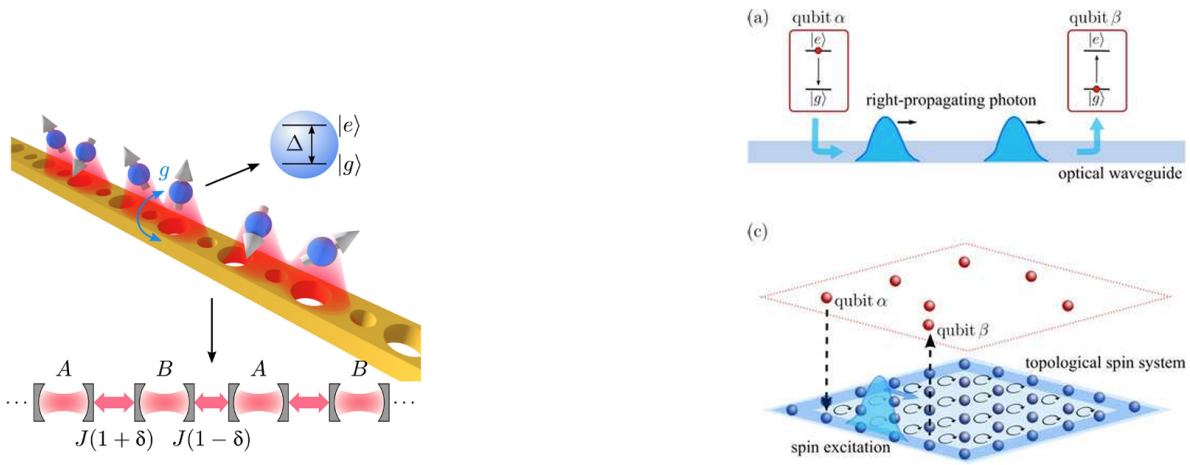


Figure 4.3: Information transfer through quantum channels composed of TLS

4.2 The Spin-Boson model and the vibrational driven model

The Spin-Boson model serves as a foundational framework for explaining the interactions between an open quantum system, specifically two-level systems (TLS), and its bosonic environment. Beyond offering a thorough and manageable portrayal of essential phenomena like quantum entanglement and decoherence, it is applicable to various fields, as noted in the introduction. In the next subsection, we will give a brief overview of this model. For those seeking a more in-depth discussion, please refer to [74].

4.2.1 Pesentation of the full quantum model.

Let us consider a simple version of the Spin-Boson model, consisting of a chain of N coupled two-levels systems (1/2-spins) interacting with a bath of harmonic oscillators (K bosonic modes). The dynamics of this open quantum system is governed by the Schrödinger equation

$$\mathbf{i}\hbar\partial_t\psi = H\psi,$$

where the quantum state is completely described by the wave function $\psi(t)$ in the Hilbert space $H = \mathbb{C}^{2N} \otimes \mathcal{F}$ where $\mathcal{F}$ is a boson Fock space. The Hamiltonian of the whole system consisting of three components, corresponding to the dynamics of the central spin-chain ($\mathcal{S}$), the vibrational bosonic environment ($\mathcal{E}$) as well as the interaction between these two subsystems ($\mathcal{I}$), and writes

$$H = H_{\mathcal{S}} \otimes \mathbb{I}_{\mathcal{F}} + \mathbb{I}_{\mathbb{C}^{2N}} \otimes H_{\mathcal{E}} + H_{\mathcal{I}}\,, \tag{4.1}$$

with

$$H_{\mathcal{S}} := \frac{\hbar}{2}\sum_{l=1}^{N}\omega_l\sigma_l^z + \sum_{l=1}^{N-1}\lambda_l\left(\sigma_l^+\,\sigma_{l+1}^- + \sigma_l^-\,\sigma_{l+1}^+\right), \quad H_{\mathcal{E}} := \hbar\sum_{k=1}^{K}\omega_{ho,k}\left(\mathbf{a}_k^\dagger\,\mathbf{a}_k + \frac{1}{2}\,Id\right), \tag{4.2}$$

and

$$H_{\mathcal{I}} := \frac{\hbar}{2}\sum_{k=1}^{K}\sum_{l=1}^{N}\sigma_l^z\left(g_{lk}\,\mathbf{a}_k^\dagger + g_{lk}^*\,\mathbf{a}_k\right).$$

For the definition of these three Hamiltonians, it is useful to index an operator acting only on the l^{th} two-level system by l, as follows

$$\sigma_l^z := \Pi_{i=1}^{l-1}\mathbb{I}_i^{\mathbb{C}^2} \otimes \sigma_z \otimes \Pi_{i=l+1}^{N}\mathbb{I}_i^{\mathbb{C}^2}\,, \quad \forall l = 1, \cdots, N\,,$$

and for $l < j$ to define

$$\sigma_l^+\sigma_j^- := \Pi_{i=1}^{l-1}\mathbb{I}_i^{\mathbb{C}^2} \otimes \sigma^+ \otimes \Pi_{i=l+1}^{j-1}\mathbb{I}_i^{\mathbb{C}^2} \otimes \sigma^- \otimes \Pi_{i=j+1}^{N}\mathbb{I}_i^{\mathbb{C}^2},$$

where $\sigma^\pm := \frac{\sigma_x \pm \mathbf{i}\,\sigma_y}{2}$ are the raising ($+$) resp. lowering ($-$) operator of the corresponding two-level atoms and $\mathbb{I}_i^{\mathbb{C}^2}$ is the identity operator on $\mathbb{C}^2$. The action of the operator $\sigma_l^+\,\sigma_j^-$ is the increase of the spin at position l and the lowering of the spin at position j. We recall here for completeness the standard complex Pauli matrices σ_x, σ_y and σ_z, given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Furthermore, we denote by λ the strength of the interaction (of dipole-dipole type) between two neighbouring TLS, by $\hbar\omega_l$ the transition energy between ground and excited state of the l^{th} TLS and by ω_{ho} the quantum harmonic oscillator's frequency, where $\mathbf{a}$ resp. $\mathbf{a}^\dagger$ are the so-called phonon annihilation resp. creation operators. Finally g_l is the interaction strength between the TLS and the bath. As explained in [73], we shall restrict this study to the single-excitation subspace and also assume that the molecules are sufficiently distant from each other, so that their mutual dipole interactions can be reduced to the dominant interaction between neighboring molecules.
For a more detailed explanation of this fully quantum model, we refer the interested reader to the first part of this work [73], where it was used to study the influence of a bath environment on excitation transfer. The distinctive feature of this dephasing model is that there is no relaxation between the spin-chain and the environment. Indeed, due to $[H_{\mathcal{I}}, \sigma_z] = 0$„ which yields $[H_{\mathcal{I}}, H_{\mathcal{S}}] = 0$, the excitation is conserved, so that decoherence is induced here by dephasing only, a situation where we deal with entropy exchange rather than energy exchange.

4.2.2 Different mathematical descriptions.

Various mathematical frameworks are available for describing the behavior of open quantum systems. The three methods listed below vary with respect to their viewpoint, complexity, and accuracy. For further insights, readers are referred to the studies [58, 64] and the citations therein. In an initial study [73], the author examined a purely quantum model to delve into how the environment affects coherent excitation transfer. However, due to computational limitations, the model was overly simplistic and didn't provide a definitive conclusion. In the subsequent research, the author employs a mixed classical-quantum model, opting to simplify the environmental component by incorporating time-dependence into the Hamiltonian.

The quantum description of the complete "central system + environment" (considered as a single quantum entity) is based on the Schrödinger equation or the equivalent von Neumann equation for pure states

$$\mathbf{i}\hbar\,\partial_t\psi = H\,\psi \quad \text{resp.} \quad \mathbf{i}\hbar\,\partial_t\rho = [H,\rho]\,, \tag{4.3}$$

where H is the full quantum Hamiltonian given in (4.1), and where ψ is the wave function describing both central system and environment with associated density matrix $\rho := |\psi\rangle\langle\psi|$, using the bra-ket notation.

The knowledge of the dynamics of the environment is not so meaningful, essential is rather its influence on the central system. To render the numerical computations more tractable, one can then reduce the problem by tracing over the environment, and considering only the central system dynamics. This average over environmental degrees of freedom leads to the problem

$$\mathbf{i}\hbar, \partial_t\rho_{\mathcal{S}} = tr_{\mathcal{E}}\,[H,\rho]\,, \qquad \rho_{\mathcal{S}} = tr_{\mathcal{E}}(\rho),.$$

At this point, it is essential to determine the processes involved, which can be characterized using a Markovian master equation [85]

$$\mathbf{i}\hbar\,\partial_t\rho_{\mathcal{S}} = \mathcal{L}\,\rho_{\mathcal{S}}\,, \tag{4.4}$$

with $\mathcal{L}$ a Linblad super-operator which incorporates the effects of the environment. The Master equation gives the evolution of an open quantum system, replacing the von Neumann equation (4.3) for isolated systems. Akin to classical mechanics, the transition from the microscopic realm to a macroscopic framework (achieved through time-scale separation and averaging) mirrors the shift from the "Langevin equation" to the "Fokker-Planck equation" in classical statistical mechanics.

In numerous instances, the irreversible behavior of an open quantum system can be described completely without referencing a quantum environment. Occasionally, such dynamics are indistinguishable from a random unitary evolution, which can be attributed to classical random fluctuations. This hybrid "quantum-classical" method captures the dynamics of the open central system influenced by an external environment through the subsequent von Neumann equation (for mixed states)

$$\mathbf{i}\hbar\,\partial_t\rho_{qc} = [H_{qc}, \rho_{qc}]\,, \qquad H_{qc} := H_{\mathcal{S}} + H_{pert}\,, \qquad H_{pert} = \frac{\hbar}{2}\sum_{l=1}^{N}\eta_l(t)\sigma_l^z\,,$$

In this context, $H_{\mathcal{S}}$ denotes the standard central system Hamiltonian (4.1), whereas H_{pert} refers to the perturbation Hamiltonian. The latter characterizes the effect of an external, macroscopic, and classical environment on the central system, characterized by some random classical noises such as stochastic Gaussian fields $\eta_l(t)$. It is necessary to juxtapose this mixed quantum-classical equation with the analogous quantum Master equation (4.4). To establish the mixed quantum-classical quantum $\leftrightarrow$ equivalence (if it exists), one must be able to identify a suitable perturbation Hamiltonian (or equivalently, appropriate stochastic fields $\eta_l(t)$) such that $\rho(t) = \rho_{qc}(t)$ for all time points. This equivalence is far from straightforward, and not every quantum model has a classical counterpart. Finding such an equivalence would imply that while the dynamics of isolated quantum systems is entirely deterministic, open quantum systems exhibit stochastic characteristics. Consequently, a dephasing environment's impact on the system of interest would be limited to the introduction of stochastic disturbances in the eigenvalues of the central system.

4.2.3 A driven excitation energy transfer model

The present paper is based on a hybrid quantum-classical model for describing the quantum excitation energy transfer (EET) in a spin-chain (photosynthesis complex), where the spins undergo classical mechanical oscillations, corresponding to the thermal vibrations of the underlying molecular structure. One important point to be investigated is the question if an ingenious choice of the underlying mechanical motion (external frequency) can enhance the EET.

Let us start with the model presented in subsection 4.2.1, however we shall not consider the interaction of our spin-chain with a random, noisy, dephasing environment. Instead we shall rather concentrate on the coherent excitation energy transfer in a spin-chain embedded in a *vibrational classical environment*, whose effect is to introduce an oscillatory motion of the molecules constituting the spin-chain (see Fig. 4.4). Hence, the dynamics

of the wave function Ψ is governed by Schrödinger's equation

$$\mathbf{i}\hbar\,\partial_t\Psi(t) = H_{\mathcal{S}}(t)\,\Psi(t)\,, \qquad \forall t>0\,, \tag{4.5}$$

where $H_{\mathcal{S}}(t)$ is of the form (4.2), however with time-dependent coupling coefficients $\lambda_l(t)$. We shall start at instant $t=0$ from the configuration of an absorbed excitation by the first two-level system, whereas all other spins are in the ground state. In the single-excitation framework, the participating configurations are regrouped in a spinor wave function

$$\Psi\in\mathbb{C}^N\,, \qquad \Psi(t) := (\psi_l(t))_{l=1}^N\,, \qquad \psi_l(t) = \psi_{---\cdots-+-\cdots-}\,,$$

where the $+$ sign represents the excited state and the wave-function $\psi_l(t)$ corresponds to the configuration with the excitation localized at the l^{th} atom.

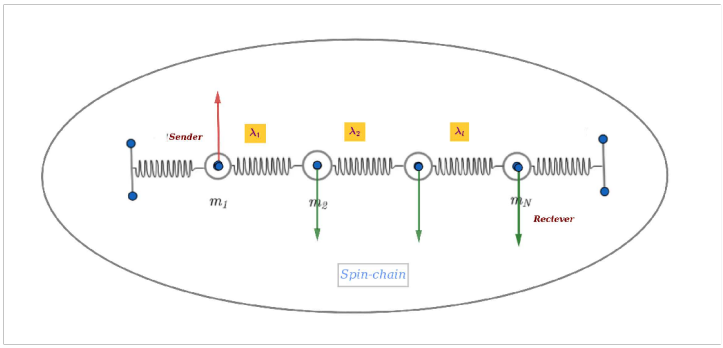


Figure 4.4: Sketch of the considered spin-chain, embedded in an exteriour vibrational environment. The first TLS is initially excited, and this excitation is then transferred towards the receiver.

In [73], constant (in time) transition energies ω_l and constant coupling coefficients λ_l are considered. However, the vibrational motion of the underlying molecular structure induces a time dependence of these coefficients and hence a time-dependent Hamiltonian $H_{\mathcal{S}}(t)$. In fact, the vibrations of the molecules change the relative distances between the two-level systems, and thus the distance-dependent dipole couplings λ_l. At the same time, small changes in the positions of the molecules can also induce modulation of the transition energies ω_l, due to the fact that these two-level systems can be immersed in a space-dependent magnetic field $\mathbf{B}(x)$. This last point will be, however, not considered here.

Denoting by $z_l(t)$ the displacements of the molecules with respect to their equilibrium positions, the distance between the l^{th} and the $(l+1)^{th}$ spin is given by

$$d_l(t) := d_0 - [z_l(t) - z_{l+1}(t)]\,, \qquad \forall t>0\,, \quad l=1,\cdots,N-1\,,$$

where $d_0>0$ is the constant equilibrium distance between the spins. For example a driven, simple sinusoidal motion, with vibrational frequency $\omega_v>0$, is described by

$$d_l(t) := d_0\,[1-2a_l\,\sin(\omega_v\,t+\varphi_l)]\,, \qquad \forall t>0\,, \quad l=1,\cdots,N-1\,, \tag{4.6}$$

with a_l the amplitude and φ_l the phase of the individual sites. A different driving motion, mainly used in engineering applications, is given under the form of a Gaussian wave-packet

$$d_l(t) := d_0\left[1-a\,e^{-\frac{[(l-1)d_0-vt]^2}{2\,\sigma^2}}\right]\,, \qquad \forall t>0\,, \quad l=1,\cdots,N-1\,, \tag{4.7}$$

with $\sigma > 0$ the pulse width, $a > 0$ the amplitude and v the velocity of the wave-packet. This motion corresponds to an exteriour guiding of the underlying molecular displacements, under the form of a pulse which propagates along the spin-chain, with its center at the position $ld_0 = vt + d_0$. The effect of the pulse is to concentrate the molecules in a certain region of the chain (which moves) and thus to couple more strongly these molecules, whereas the coupling of the rest part of the chain remains unaffected. This type of external guiding shall however not be treated in this chapter, we shall rather focus on the oscillatory motion (4.6).

The coupling strengths $\lambda_l(t)$ are now imposed by the distances between the neighbouring spins, via the formula (dipole-dipole interactions)

$$\lambda_l(t) := \frac{\tilde{\lambda}_l}{[d_l(t)/d_0]^3}\,, \qquad \forall t > 0\,, \quad l = 1, \cdots, N-1\,,$$

where $\tilde{\lambda}_l$ are the time-independent couplings of the molecular static chain. This formula underlines the fact that the closer the TLSs are, the stronger the coupling is.

Given all these coefficients, one can solve the Schrödinger equation (4.5) and compute now the **site occupation probabilities** $\mathcal{P}_l(t)$ of the l^{th} two-level system via

$$\mathcal{P}_l(t) := |\psi_l(t)|^2\,, \quad \forall l = 1, \cdots, N\,,$$

quantities which shall permit to localize the excitation in the spin-chain, and thus to study the excitation transfer from one end-point to the other of the spin-chain. These probability functions depend naturally on $\{\lambda_l(t)\}_{l=1}^{N-1}$ and hence on the external mechanical frequency ω_v. Thus, an effective interplay between the mechanical oscillations (ω_v) on one hand, and the eigen-frequencies of the non-perturbed spin-chain (ω_l for $l = 1, \cdots, N$) on the other hand, could improve the excitation energy transfer. Our aim is to tune the model in such a manner to get a perfect excitation energy transfer in the shortest possible time $t_\sharp$ (*i.e.* $\mathcal{P}_N(t_\sharp) = 1$).

To summarize, the hybrid model presented here is based on a cooperative interplay between the quantum coherent dynamics of the excitation along the spin-chain and the mechanical classical vibration of the underlying molecules. The Hamiltonian governing the quantum excitation motion will acquire a time-dependence, induced by the deterministic motion of the molecular structure, which is a consequence of the thermal classical environment. This leads necessarily to a driven coherent excitation dynamics (Rabi oscillations), which shall be tuned to get an efficient excitation energy transfer from the first to the last two-level system of the spin-chain.

4.2.4 Analytical solutions in some specific situations

Our aim is now to understand how the information (or excitation) is transferred within the spin chain. We recall that we are interested in the case where only one excitation is allowed in the whole chain. To obtain the dynamics of this excitation, one has to solve the Schrödinger equation (4.5). Even if this linear equation looks simple, it is in general not possible to obtain analytical solutions when the interaction coefficients $\{\lambda_l(t)\}_{l=1}^{N-1}$ are

time-dependent. There are however situations for which this Schrödinger equation can be solved analytically, situations we shall explicit in this subsection.
For this we decompose the Hamiltonian into the constant, diagonal unperturbed spin-chain part H_0, and the time-depending, hermitian interaction part $H_{int}(t)$, namely

$$H_{\mathcal{S}}(t) := H_0 + H_{int}(t) = \begin{pmatrix} \epsilon_1 & 0 & 0 & 0 \\ 0 & \epsilon_2 & 0 & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \epsilon_N \end{pmatrix} + \begin{pmatrix} 0 & \lambda_1(t) & 0 & 0 \\ \lambda_1^*(t) & 0 & \lambda_2(t) & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \lambda_{N-1}^*(t) & 0 \end{pmatrix},$$

with the eigenstates of H_0 (energy-levels of the different possible configurations in our unperturbed spin-chain) given by

$$\epsilon_l := \frac{\hbar}{2} \sum_{j=1}^{N} s_j^{(l)} \omega_j \,,$$

where $s_j^{(l)} := \pm 1$ is the sign of the j^{th} atom in the l^{th} configuration, namely $+1$ for the excited state and -1 for the ground state. The first Hamiltonian H_0 incorporates the energies of the quantum spin-chain in the absence of the spin interactions. The second Hamiltonian $H_{int}(t)$ describes the interaction of the spin-chain with the vibrational environment. The fact that $H_{int}(t)$ is not diagonal leads to transitions between the different eigenstates of H_0.

Filtering out the diagonal part, the solution of the Schrödinger equation (4.5) can now be expressed as

$$\Psi(t) = \Sigma_{l=1}^{N} \alpha_l(t) e^{-\mathbf{i}\epsilon_l t/\hbar} \, \mathbf{e}_l \,, \qquad H_0 \, \mathbf{e}_l = \epsilon_l \, \mathbf{e}_l \,, \tag{4.8}$$

called also *interaction representation* of the wave-function, and where $\{\epsilon_l, \mathbf{e}_l\}_{l=1}^N$ are the eigenvalues resp. eigenvectors of H_0. Inserting Ansatz (4.8) into (4.5) permits to get a coupled ODE system for the expansion coefficients $\alpha_l(t)$, namely

$$\begin{pmatrix} \alpha_1'(t) \\ \alpha_2'(t) \\ \vdots \\ \alpha_N'(t) \end{pmatrix} = -\frac{\mathbf{i}}{\hbar} \begin{pmatrix} 0 & \lambda_1(t) e^{-\mathbf{i}(\epsilon_2-\epsilon_1)t/\hbar} & & 0 \\ \lambda_1^*(t) e^{\mathbf{i}(\epsilon_2-\epsilon_1)t/\hbar} & 0 & \lambda_2(t) e^{-\mathbf{i}(\epsilon_3-\epsilon_2)t/\hbar} & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \lambda_{N-1}^*(t) e^{\mathbf{i}(\epsilon_N-\epsilon_{N-1})t/\hbar} & 0 \end{pmatrix} \begin{pmatrix} \alpha_1(t) \\ \alpha_2(t) \\ \vdots \\ \alpha_N(t) \end{pmatrix}. \tag{4.9}$$

In the absence of interaction $\lambda_l(t) \equiv 0$ for all $l = 1, \cdots N$, we immediately observe that the coefficients $\alpha_l(t)$ are constant in time, which signifies simply that we are in the situation of a stationary solution, with time-independent occupation probabilities. At this point, the idea is now to try to solve system (4.9). Unfortunately this apparently very simple ODE system cannot be solved analytically in general, and numerical simulations are the only rescue. Explicit computations can be done however in some specific situations we shall precise now, in order to get a feeling of the phenomenon of driven excitation energy

transfer.

For example in the case one considers equal, but time-dependent coupling coefficients $\lambda_l(t) \equiv \lambda(t)$, and uniform local energy-levels $\varepsilon_l = \varepsilon$, the computation of the solutions to the Schrödinger equation (4.5) is trivial. The eigenvalues resp. eigenvectors of the Hamiltonian $H_{\mathcal{S}}$ are given in this case by

$$E_l(t) := \varepsilon + 2\,\lambda(t)\,\cos\left(\frac{\pi\,l}{N+1}\right)\,, \qquad \phi_l = \sqrt{\frac{2}{N+1}}\,\sum_{j=1}^{N}\sin\left(\frac{\pi\,l\,j}{N+1}\right)\,\mathbf{e}_j\,, \quad l = 1, \cdots, N\,,$$

and the solution to $\mathbf{i}\hbar\,\partial_t\Psi(t) = H_{\mathcal{S}}\Psi(t)$, with initial condition $\Psi(0) = \mathbf{e}_1$, takes the form

$$\Psi(t) = \Sigma_{l=1}^{N}\beta_l\,e^{-\mathbf{i}\mathfrak{E}_l(t)/\hbar}\,\phi_l\,, \quad \beta_l = \sqrt{\frac{2}{N+1}}\,\sin\left(\frac{\pi\,l}{N+1}\right)\,, \quad l = 1, \cdots, N\,,$$

if we integrate $E_l(t)$, for $l = 1, \cdots, N$, we get

$$\mathfrak{E}_l(t) = \varepsilon\,t + \mu_l\,\Lambda(t)\,, \qquad \mu_l := 2\,\cos\left(\frac{\pi\,l}{N+1}\right)\,, \quad \Lambda(t) := \int_0^t \lambda(s)\,ds\,.$$

This yields for each component of the wave-function the exact expression

$$\psi_k(t) = \frac{2}{N+1}e^{-\mathbf{i}\,\varepsilon\,t/\hbar}\sum_{l=1}^{N}\left[\sin\left(\frac{\pi l}{N+1}\right)\sin\left(\frac{k\pi l}{N+1}\right)e^{-\mathbf{i}\mu_l\Lambda(t)/\hbar}\right], \qquad k = 1, \ldots, N$$

and in particular for the last spin-up configuration ($k = N$)

$$\psi_N(t) = -\frac{2}{N+1}\,e^{-\mathbf{i}\,\varepsilon\,t/\hbar}\,\sum_{l=1}^{N}(-1)^l\,\sin^2\left(\frac{\pi\,l}{N+1}\right)\,e^{-\mathbf{i}\mu_l\Lambda(t)/\hbar}\,.$$

The occupation probability of each spin $k = 1, \ldots, N$ is then given by

$$\begin{aligned}\mathcal{P}_{k,N}(t) = 2\,\tfrac{4}{(N+1)^2}\,\Sigma_{l=1}^{N}\,\Sigma_{h<l}\,\sin\left(\tfrac{\pi\,l}{N+1}\right)\,\sin\left(\tfrac{\pi\,kl}{N+1}\right)\,\sin\left(\tfrac{\pi\,h}{N+1}\right)\,\sin\left(\tfrac{\pi\,hk}{N+1}\right)\,*\\ *\,\cos\left(\tfrac{2}{\hbar}\,\Lambda(t)\,\left[\cos\left(\tfrac{\pi\,l}{N+1}\right) - \cos\left(\tfrac{\pi\,k}{N+1}\right)\right]\right) + \tfrac{4}{(N+1)^2}\,\Sigma_{l=1}^{N}\,\sin^4\left(\tfrac{\pi\,l}{N+1}\right)\,,\end{aligned}$$

in particular, one has for the last spin ($k = N$)

$$\begin{aligned}\mathcal{P}_N(t) = 2\,\tfrac{4}{(N+1)^2}\,\Sigma_{l=1}^{N}\,\Sigma_{k<l}(-1)^{l+k}\,\sin^2\left(\tfrac{\pi\,l}{N+1}\right)\,\sin^2\left(\tfrac{\pi\,k}{N+1}\right)\,*\\ *\,\cos\left(\tfrac{2}{\hbar}\,\Lambda(t)\,\left[\cos\left(\tfrac{\pi\,l}{N+1}\right) - \cos\left(\tfrac{\pi\,k}{N+1}\right)\right]\right) + \tfrac{4}{(N+1)^2}\,\Sigma_{l=1}^{N}\,\sin^4\left(\tfrac{\pi\,l}{N+1}\right)\,.\end{aligned} \tag{4.10}$$

What can be observed from these formulae is that the effect of the magnitude of a constant coupling strength λ is nothing but a time-scaling. Furthermore, we can check that the excitation transfer is no more fully achieved for $N > 3$ and constant λ, in particular the probability of the excitation to reach the final spin reduces with the length of the chain, the reason being the dispersion of the initial excitation over the whole chain (see [59] and Figure 4.5). For $N = 3$ one prove the following property.

Lemma 4.2.1. *If we consider driven model for three spins ($N = 3$) and equal, positive as well as time-depending coupling coefficients, $\lambda(t) > 0$, then there exists a time $t_\sharp > 0$ at which the occupation probability $\mathcal{P}_3(t)$, which reads*

$$\mathcal{P}_3(t) = \sin^4\left(\frac{1}{\sqrt{2}\hbar}\Lambda(t)\right) \qquad \forall t > 0,$$

is equal to one, thus we have complete excitation transfer in a finite time.

Proof. Using formula (4.10) one gets

$$\mathcal{P}_3(t) = \frac{1}{4}\cos^2\left(\frac{\sqrt{2}}{\hbar}\Lambda(t)\right) - \frac{1}{2}\cos\left(\frac{\sqrt{2}}{\hbar}\Lambda(t)\right) + \frac{1}{4} = \frac{1}{4}\left[\cos\left(\frac{\sqrt{2}}{\hbar}\Lambda(t)\right) - 1\right]^2, \qquad \forall t > 0.$$

Thus

$$P_3(t_\sharp) = 1 \iff \cos\left(\frac{\sqrt{2}}{\hbar}\Lambda(t_\sharp)\right) = -1 \iff \Lambda(t_\sharp) = \frac{(2k+1)\pi\hbar}{\sqrt{2}}, \quad \forall k \in \mathcal{N}.$$

As $\Lambda'(t) = \lambda(t) > 0$, the functional $\Lambda(t)$ is strictly increasing, starting from $\Lambda(0) = 0$, such that one can find several complete transfer times $t_\sharp^{(k)} := \Lambda^{-1}\left(\frac{(2k+1)\pi\hbar}{\sqrt{2}}\right) > 0$ for each $k \in \mathcal{N}$, for which $\mathcal{P}_3(t_\sharp^{(k)}) = 1$. □

These computations become difficult in the time-dependent general case $(\epsilon_l, \lambda_l(t))_{l=1}^N$ and we shall turn in subsection 4.3.2 towards numerical methods.

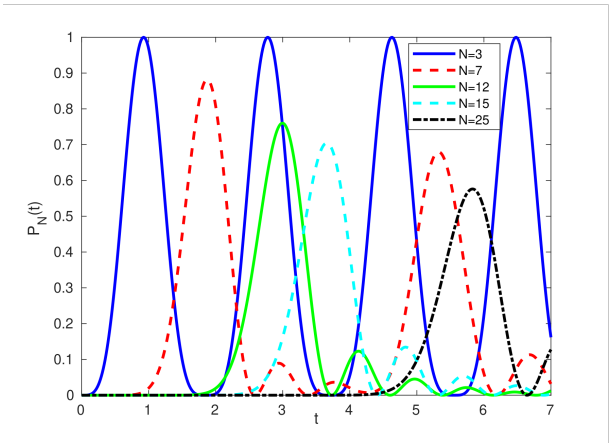


Figure 4.5: Plot of the time-evolution of the occupation probability $\mathcal{P}_N(t)$, for several $N = 3, 7, 12, 15, 25$ and constant coupling strength $\lambda = 2.4$.

4.3 Study of the vibrational induced enhancement of the excitation transfer

4.3.1 Driven model for two spins

Let us investigate in this subsection a chain constituted of only two spins and examine the occupation probabilities $\{\mathcal{P}(t)\}_{l=1}^{2}$ in order to understand in more details in this simplified framework the influence of the mechanical vibration on the quantum excitation energy transfer. Denoting by $Z(t) := (\alpha_1(t), \alpha_2(t))^{\mathbf{t}}$ the coefficients arising in (4.8), we have to solve

$$Z'(t) = -\frac{\mathbf{i}}{\hbar}\lambda(t)\begin{pmatrix} 0 & e^{-\mathbf{i}\omega_c t} \\ e^{\mathbf{i}\omega_c t} & 0 \end{pmatrix} Z(t)\,, \qquad \omega_c := \frac{\epsilon_2 - \epsilon_1}{\hbar}\,, \tag{4.11}$$

for an initial condition $Z(0) = (1,0)^{\mathbf{t}}$. The parameter $\omega_c > 0$ represents the transition frequency between the two energy-levels of the system. An explicit solution to (4.11) can be found only in some specific situations, we shall study now.

Constant coefficient case: $\lambda > 0$ and $\omega_c \equiv 0$.

In the case of constant coupling coefficients and equal energy levels $\varepsilon_l = \varepsilon$ one can easily compute the occupation probabilities via (4.10), yielding

$$\mathcal{P}_1(t) = |\psi_1(t)|^2 = \cos^2\left(\frac{\lambda\, t}{\hbar}\right), \qquad \mathcal{P}_2(t) = |\psi_2(t)|^2 = \sin^2\left(\frac{\lambda\, t}{\hbar}\right), \quad \forall t > 0\,.$$

A beating phenomenon is observed, the excitation is transferred regularly forth and back between the first and the second TLS, with an angular frequency of $\omega_R := 2\frac{\lambda}{\hbar}$. This phenomenon is known as *Rabi oscillations* (see Fig. 4.6). Rabi oscillations are a quantum mechanical phenomenon in which a two-level system undergoes periodic oscillations between its states when exposed to an external resonant electromagnetic field. Essentially, the Rabi phenomenon describes the continuous exchange of energy between the quantum system and the driving field, leading to observable oscillations in the population of the two levels.
Coming back to our spin-chain, we have always in this situation a perfect transfer from site one towards site two, with a transfer time of $t_\sharp = \frac{\hbar}{2\lambda}$, which decreases with the increase of the coupling strength. In order to catch the excitation at the end-point of the spin-chain, one has to know exactly when this excitation arrived at destination, this knowledge being crucial for applications.

Constant coupling $\lambda > 0$, different energy levels $\omega_c \neq 0$.

The situation is different when the energy-levels are not any more equal. In this case, there is no more full excitation transfer. Indeed, one can compute analytically in this case the solution to (4.11), yielding for all $t > 0$

$$\mathcal{P}_1(t) = \frac{(\lambda/\hbar)^2}{(\lambda/\hbar)^2 + (\omega_c/2)^2}\cos^2\left(\frac{\omega_R}{2}\,t\right) + \frac{\omega_c^2}{\omega_R^2}\,, \qquad \mathcal{P}_2(t) = \frac{(\lambda/\hbar)^2}{(\lambda/\hbar)^2 + (\omega_c/2)^2}\sin^2\left(\frac{\omega_R}{2}\,t\right),$$

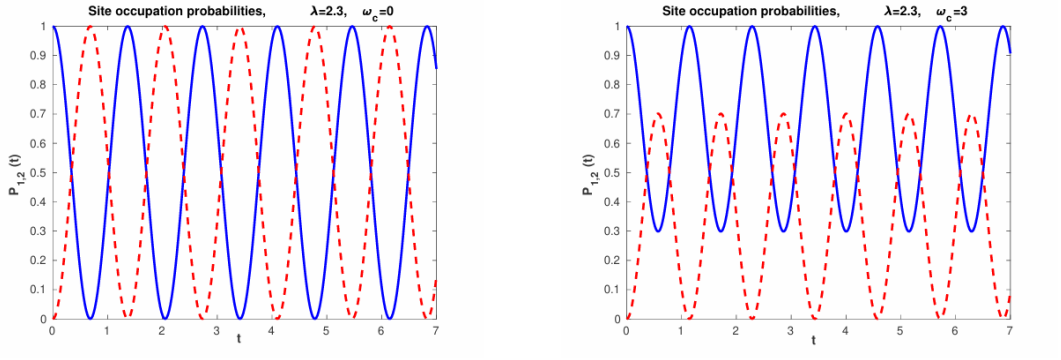


Figure 4.6: Site occupation probability $\mathcal{P}_1(t)$ in blue (full line) resp. $\mathcal{P}_2(t)$ in red (dashed line), for a constant coupling strength $\lambda = 2, 3$. Left:$\omega_c = 0$. Right: $\omega_c = 3$.

where ω_R is the so-called (angular) Rabi-frequency, defined as

$$\omega_R^2 := 4\,(\lambda/\hbar)^2 + \omega_c^2\,.$$

One can observe that the excitation oscillates forth and back, with Rabi-frequency ω_R and an amplitude of $\frac{(\lambda/\hbar)^2}{(\lambda/\hbar)^2+(\omega_c/2)^2}$,which never reaches one for $\omega_c \neq 0$. Even if the transfer is not perfect, its transfer time is given by $t_\sharp = \frac{\pi}{\omega_R}$. In the limit of vanishing ω_c, or strong coupling strength, meaning for $\hbar\omega_c << 2\lambda$ one gets exactly the previous case

$$\lim_{\frac{\hbar\omega_c}{2\lambda}\to 0} \mathcal{P}_2(t) = \sin^2\left(\frac{\lambda\, t}{\hbar}\right), \qquad \lim_{\frac{\hbar\omega_c}{2\lambda}\to 0} t_\sharp = \frac{\hbar\pi}{2\lambda}.$$

See right of Fig. 4.6 for the occupation probabilities $\mathcal{P}_{1,2}(t)$ in a case of a constant coupling strength $\lambda = 2.3$ and non-vanishing $\omega_c = 3$.

Time-varying coupling $\lambda(t)$ and equal energy levels $\omega_c \equiv 0$.

Coming now to the time-dependent case (4.11) with $\omega_c \equiv 0$, the **site occupation probabilities** $\{\mathcal{P}(t)\}_{l=1}^2$ are given via (4.10) by

$$\mathcal{P}_1(t) = \cos^2\left(\frac{1}{\hbar}\int_0^t \lambda(s)\,ds\right), \qquad \mathcal{P}_2(t) = \sin^2\left(\frac{1}{\hbar}\int_0^t \lambda(s)\,ds\right). \tag{4.12}$$

The interpretation of these formulae is more delicate and to make concepts more concrete, we shall perform several numerical tests with specific $\lambda(t)$,in the aim to study the excitation transfer.
But before, let us start by making some observations. Firstly, recall that the coupling coefficient $\lambda(t)$ relies on the distance between the molecules of the chain (see expression (4.7)), and hence depends on the frequency ω_v of the underlying vibrational motion of the molecules. Now, a tricky coordination between the mechanical oscillation frequency ω_v and the Rabi frequency ω_R of the macroscopic oscillations may be beneficial for a quick and complete transfer of the excitation between site one and site two. To be more precise,

take a look at formula (4.12) and remark for example that the period of the integrand $\lambda(s)$ is $T_v = \frac{2\pi}{\omega_v}$. If the vibrational motion is now synchronized such that one gets the relation $\frac{1}{\hbar}\int_0^{T_v} \lambda(s)ds = \pi$, then the probabilities $\{\mathcal{P}_l(t)\}_{l=1}^2$ are T_v-periodic with Rabi frequency $\omega_R := \omega_v$. For periods T_v which does not satisfy such a relation, the excitation transfer is no more periodic.

Let us go into more details and investigate the effect of the specific time-depending coupling strength $\lambda(t)$, given by

$$\lambda(t) := \frac{\tilde{\lambda}}{[d(t)/d_0]^3}\,,\; d(t) := d_0\left[1-\sqrt{3}a\,\sin(\omega_v\, t+\varphi)\right],\; a = 1/(2\sqrt{3}),\; d_0 = \tilde{\lambda} = 1\,,\; \varphi = \pi/2\,, \tag{4.13}$$

on the occupation probabilities $\{\mathcal{P}_l(t)\}_{l=1}^2$, where we fixed for these tests $\hbar = 1$. In particular, we are interested in understanding the influence of the underlying vibrational frequency ω_v on the excitation transfer. Thus, to underline the dependence of λ and hence of its primitive on ω_v, let us denote

$$\Lambda(t,\omega_v) := \int_0^t \lambda_{\omega_v}(s)\,ds,$$

and study some of its properties in the next lemma.

Lemma 4.3.1. *The function*

$$\Lambda(t,\omega_v) := \int_0^t \frac{8}{[2-\cos(\omega_v s)]^3}\,ds,$$

is strictly increasing in t, namely $\partial_t\Lambda(t,\omega_v) > 0$ for all ω_v, and satisfies moreover

$$\lim_{\omega_v\to+\infty}\Lambda(t,\omega_v) = \gamma\, t, \qquad \gamma := \frac{1}{T_{\omega_v}}\int_0^{T_{\omega_v}} \frac{8}{[2-\cos(\omega_v s)]^3}\,ds = \frac{4}{\sqrt{3}}, \quad \forall t>0,$$

with $T_{\omega_v} := \frac{2\pi}{\omega_v}$. Thus, one has for the occupation probabilities

$$\mathcal{P}_2(t_\sharp) = \sin^2\!\left(\frac{1}{\hbar}\Lambda(t_\sharp,\omega_v)\right) = 1 \iff \Lambda(t_\sharp^{(k)},\omega_v) = \frac{(2k+1)\pi\hbar}{2}, \quad \forall k\in\mathcal{N},$$

leading to a ω_v-dependent transfer time, which is oscillating in ω_v and satisfies (for $k=1$)

$$t_\sharp(\omega_v) \to_{\omega_v\to\infty} \frac{\pi\hbar}{2\gamma} = \frac{\sqrt{3}}{8}\pi\hbar \simeq 0,68.$$

Remark 4.3.1. To vizualize the properties of this Lemma, we plotted on Figure 4.7 the phase factor $\Lambda(t,\omega) := \int_0^t \lambda(s)\,ds$, as a function of time, and this for different ω_v-values, as well as the excitation transfer time $t_\sharp(\omega_v)$, for which $\mathcal{P}_2(t_\sharp(\omega_v)) = 1$.

Proof. A simple change of variable yields (denoting $\omega_v = \omega$ for simplicity)

$$\Lambda(t,\omega) = \frac{1}{\omega}\int_0^{\omega t} \frac{8}{[2-\cos(\tau)]^3}\,d\tau.$$

Assuming now that $\omega t \in [2k\pi, 2(k+1)\pi)$ for some $k \in \mathbb{N}$, permits to show that

$$\Lambda(t,\omega) \leq \frac{t}{2\pi}\int_0^{2\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau + \frac{1}{\omega}\int_0^{2\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau = \left(\frac{t}{2\pi}+\frac{1}{\omega}\right)\frac{8\pi}{\sqrt{3}},$$

therefore

$$\lim_{\omega\to+\infty} \Lambda(t,\omega) \leq \frac{4t}{\sqrt{3}}.$$

In the same way

$$\begin{aligned}\Lambda(t,\omega) &= \frac{k+1}{\omega}\int_0^{2(k+1)\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau - \frac{1}{\omega}\int_{\omega\, t}^{2(k+1)\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau \\ &\geq \frac{t}{2\pi}\int_0^{2\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau - \frac{1}{\omega}\int_0^{2\pi} \frac{8}{[2-\cos(\tau)]^3}\,d\tau = \left(\frac{t}{2\pi}-\frac{1}{\omega}\right)\frac{8\pi}{\sqrt{3}},\end{aligned}$$

hence

$$\lim_{\omega\to+\infty} \Lambda(t,\omega) = \frac{4t}{\sqrt{3}}.$$

□

But it is not only the transfer time which is of importance for the excitation transfer from site one towards site two. Indeed, another important aspect to be investigated is the time the transferred excitation spends on the second site. A tricky modulation of the coupling strength can elongate the effective time the excitation rests at site two, fact which enables this excitation to "jump" more rapidly to the next site (if the spin-chain is longer), and not to come back to the first site. This aspect, strictly related to the time-dependence of the coupling strength, will be discussed now in detail.

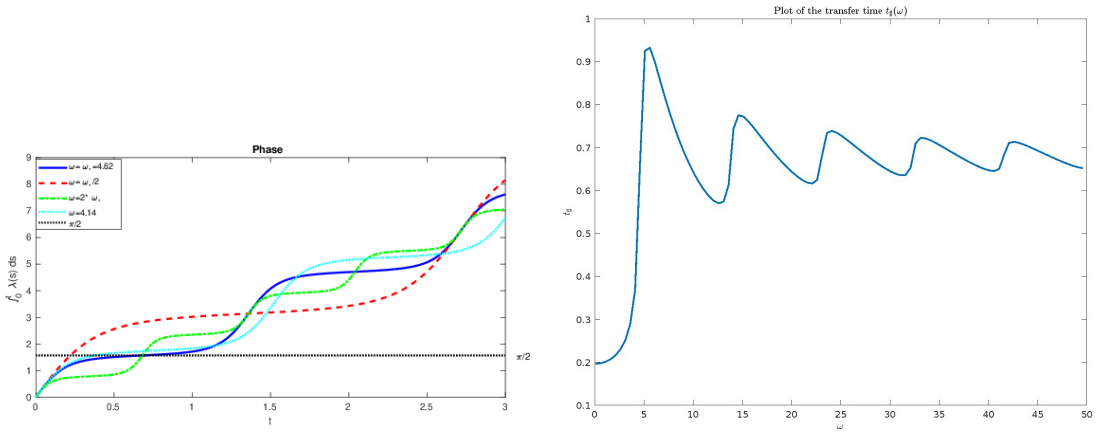


Figure 4.7: Left: Plot of the phase function $\Lambda(t,\omega_v) := \int_0^t \lambda(s)\,ds$. The plot for $\omega = \omega_\star$ corresponds to Fig. 4.8. Right: Plot of the transfer time $t_\sharp(\omega)$ with respect to the vibrational frequency ω_v

In Figure 4.8 we plotted the shape of the coupling-strength $\lambda(t)$ given in (4.13) and the corresponding site occupation probabilities. Due to the mechanical oscillations of the underlying molecular structure, the coupling of the TLS exhibits narrow regions of

strong interaction and larger regions of weaker interaction, this asymmetry is coming from the form of the dependence of $\lambda(t)$ upon the distance between the spins $d(t)$. What is expected is a faster excitation propagation between the sites whenever the coupling is stronger (meaning when two spins are closer to one another). A beating between the two spins is observed, similarly to the uniform coupling case of subsection 3.1.1, beating plotted on the right of Figure 4.8. But, contrary to the static coupling case, in the time-dependent configuration we observe the so-called *quick-transfer-and-locking-phenomenon* (term used in [51]). In other words, during the short time-interval of strong coupling, the excitation is quickly transferred from one site to the neighbouring one, whereas during the longer time-interval of weaker coupling, the excitation is locked on one site. One cannot visualize in this simple case with $N = 2$ spins the advantage of this *quick-transfer-and-locking-effect* on the excitation energy transfer, as for $N \leq 3$ the excitation is always completely transferred from the first to the last spin. However, the simple fact that, after being rapidly (and completely) transferred from spin 1 towards spin 2, the excitation remains locked at site 2 for some time, can be very advantageous. Indeed, the excitation has then a bigger probability to be carried over to a next site 3 (if the chain is longer) or to a sink, instead of being transferred back to site one. In this manner a transfer along the chain will be possible.

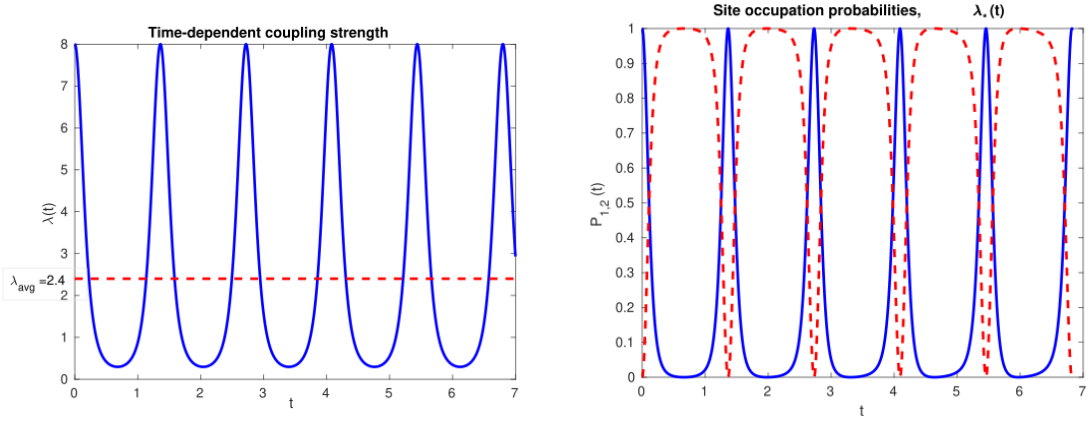


Figure 4.8: Left: Time evolution of $\lambda(t)$ for $\omega_\star = 4.62$. Right: Corresponding site occupation probabilities $\mathcal{P}_1(t)$ (full blue line) and $\mathcal{P}_2(t)$ (dashed red line).

In order to render this *quick-transfer-and-locking-phenomenon* efficient for the overall excitation transfer, a particular synchronization is required between the underlying classical oscillations and the quantum (Rabi) excitation oscillation, pictured for example by the formula of the occupation probability in the uniform energy-level case

$$\mathcal{P}_2(t) = \sin^2\left(\frac{1}{\hbar}\int_0^t \lambda(s)\,ds\right) = \sin^2\left(\frac{1}{\hbar}\Lambda(t,\omega_v)\right).$$

In this simplified case a synchronization arises when one requires that during half of the period of the mechanical oscillation $T_v/2$ the excitation is completely transferred from site one towards site two (see Fig. 4.8 for a better comprehension). This is achieved when

asking for which $\omega_\star$ (if there is one) one has

$$\Lambda(T_v/2,\omega_\star)=\int_0^{T_v/2}\lambda_{\omega_\star}(t)\,dt=\frac{\pi}{2}\hbar\quad\text{leading to}\quad\mathcal{P}_2(T_v/2)=1\,,$$

This shall permit to obtain the optimal frequency $\omega_\star$ for which the excitation spends a maximal time on the second site. To compute this optimal frequency ω_v, we use a change of variable $\theta(s):=\lambda(s/\omega_\star)$ with $\lambda(t)$ given in (4.13), leading to

$$\frac{\pi}{2}\hbar=\int_0^{T_v/2}\lambda(t)\,dt=\frac{1}{\omega_\star}\int_0^{\pi}\theta(s)\,ds\quad\Rightarrow\quad\omega_\star=\frac{2}{\pi\hbar}\int_0^{\pi}\theta(s)\,ds\approx 4.62\,.$$

One can think it could be better to ask (as in [51]) that during a quarter of the mechanical oscillation period $T_v/4$ (during which the coupling is strong, see left of Fig. 4.8) the excitation is completely transferred from site one towards site two, namely to ask rather

$$\int_0^{T_v/4}\lambda(t)\,dt=\frac{\pi}{2}\hbar\quad\text{leading to}\quad\mathcal{P}_2(T_v/4)=1\quad\text{and}\quad\tilde{\omega}=\frac{2}{\pi\hbar}\int_0^{\pi/2}\theta(s)\,ds\approx 4.14\,.$$

The occupation probabilities corresponding to $\tilde{\omega}=4.14$ are plotted on Fig. 4.9. One remarks firstly that the curves are no more periodic, and secondly that the excitation arrives more rapidly at the last spin, however it remains there not as long as for $\omega_\star=4.62$.

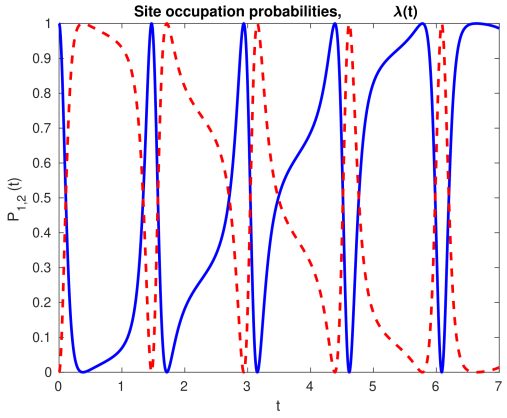


Figure 4.9: Time evolution of the site occupation probabilities $\mathcal{P}_1(t)$ (full blue line) and $\mathcal{P}_2(t)$ (dashed red line) for $\omega_v=\tilde{\omega}=4.14$.

On Figure 4.10 we plotted the site occupation probabilities for the two different vibrational frequencies $\omega_1:=\omega_\star/2$ and $\omega_2:=2\omega_\star$. When comparing these plots with the right plot of Fig. 4.8, which corresponds to the "optimal" frequency $\omega_\star$, we observe clearly a non-synchronization in these non-optimal frequencies ω_1,ω_2, which leads to a non-efficient excitation transfer within the spin-chain. Indeed, in this case one observes that the excitation, after being transferred to the second site (more or less rapidly), remains there only for a short time and is transferred back to site 1. Thus, it would not have enough time to

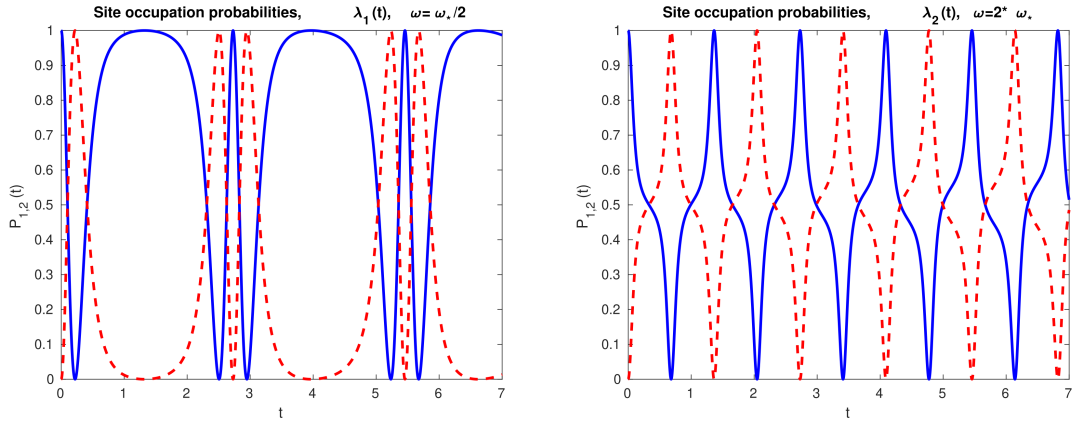


Figure 4.10: Site occupation probabilities $\mathcal{P}_{1,2}(t)$ for the two frequencies $\omega_1 = \omega_\star/2$ on the left and $\omega_2 = 2\omega_\star$ on the right.

be transferred to a further spin, if the chain was longer.

To summarize, the observed effects of a modulation of the coupling strength $\lambda(t)$ (via the underlying mechanical oscillations) in the case of a chain of $N = 2$ spins, are:

- the transfer time from one end towards the other end of the chain is ω_v-dependent, however the excitation is always completely transferred;
- the time the excitation spans on the second site is also ω_v-dependent, with a maximum for a well-identified frequency $\omega_\star$.

4.3.2 Driven model for $N = 7$ spins

For longer spin-chains, as for example when considering the coupled pigments in a photosynthesis complex constituted of $N = 7$ sites, the excitation is no more completely transferred from the first to the last spin, and this due to the dispersion of the initial excitation over the whole spin-chain. What is now expected is an improvement of the transfer by manipulating the coupling strength, via the underlying mechanical oscillations of the molecular structure. In the former paper [73], one of the authors showed that for a particular static coupling configuration given by $\lambda_l := \lambda_0 \sqrt{l(N-l)}$ one obtains a perfect excitation transfer for all possible chain lengths, however this configuration is very sensitive to exteriour perturbations. In the present chapter, we follow a different idea, introducing the inevitable vibrational motion of the underlying molecular chain into the model and investigating its influence on the excitation energy transfer.

For long spin-chains with $N \geq 3$, one cannot do any more explicit computations, and we shall present in this section some numerical results for the driven sinusoidal model, with

$$d_l(t) := d_0 - \left[z_l^{(m)}(t) - z_{l+1}^{(m)}(t) \right] , \qquad z_l^{(m)}(t) := d_0\, a\, \sin\left(\frac{m\,\pi\,l}{N+1} \right) \sin(\omega_v\, t + \varphi) ,$$

$$\lambda_l(t) := \frac{\tilde{\lambda}_l}{[d_l(t)/d_0]^3}\,, \qquad \forall t > 0\,, \quad l = 1, \cdots, N-1\,,$$

where $m = 1, \cdots, N$ corresponds to the considered normal mode and

$$\varepsilon_l \equiv 0\,, \quad a \equiv 1/4\,, \;\; d_0 = \tilde{\lambda}_l \equiv 1\,, \;\; \varphi \equiv \pi/2\,, \quad \omega_v \in [2, 10]\,.$$

Choosing the mode $m = N$ means that we are considering again the breathing mode, as for the 2-spin chain, mode which can be associated with a human chain (bucket brigade for firefighting) transferring for example a water bucket from the reservoir towards the fire (see Fig. 4.11). This mode is the most appropriate one for an efficient excitation transfer, as shall be seen in the sequel, and this again if a certain synchronization is maintained between the underlying mechanical frequency and the quantum Rabi frequency.

Figure 4.11: Human chain representing the breathing mode of our spin-chain, inspiring a bucket-brigade device for an efficient excitation transfer (http://www.sylvesterdesign.com).

The numerical simulations are based on a resolution of the ODE system (4.9) via the Crank-Nicolson method. Let us discretize the time interval $[0, T_{fin}]$ in a homogeneous manner, with $\Delta t := T_{fin}/N_t$, $t_k := k\,\Delta t$, $k = 0, \cdots, N_t$ and where $N_t \in \mathcal{N}$ is the number of time intervals. Then the ODE system (4.9), written under the more general form

$$\left\{ \begin{array}{l} Z'(t) = A(t)\,Z(t)\,, \qquad t \in (0, T_{fin}] \\ Z(0) := Z_0 \in \mathbb{R}^N\,, \end{array} \right. , \qquad Z(t) := (\alpha_1(t), \cdots, \alpha_N(t))^{\mathbf{t}}\,,$$

is approximated by the following second-order A-stable Crank-Nicolson scheme

$$\left\{ \begin{array}{l} \left[Id - \frac{\Delta t}{2}\,A(t_{k+1})\right]\,Z^{k+1} = \left[Id + \frac{\Delta t}{2}\,A(t_k)\right]\,Z^k\,, \qquad \forall k = 0, \cdots, N_t - 1 \\ Z^0 \equiv Z_0\,. \end{array} \right.$$

In order to demonstrate how the presence of an underlying mechanical vibration can enhance the EET, we shall compare now the occupation probability at the last site $\mathcal{P}_7(t)$ for different coupling-strengths $\lambda(t)$, varying the frequency ω_v of the underlying oscillations, as well as comparing the results with a static configuration (constant λ).

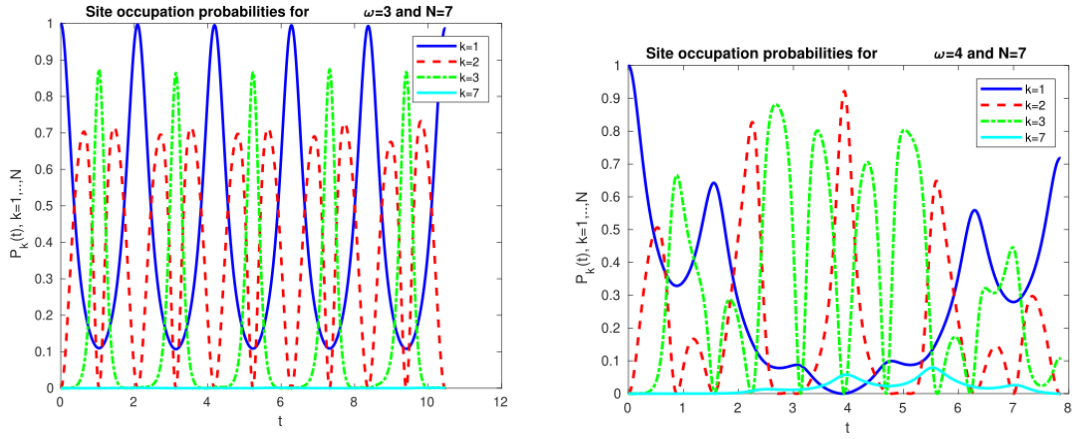


Figure 4.12: Site occupation probabilities $\mathcal{P}_k(t)$ for the two frequencies $\omega_v = 3$ and $\omega_v = 4$, and for $m = 7$, $N = 7$.

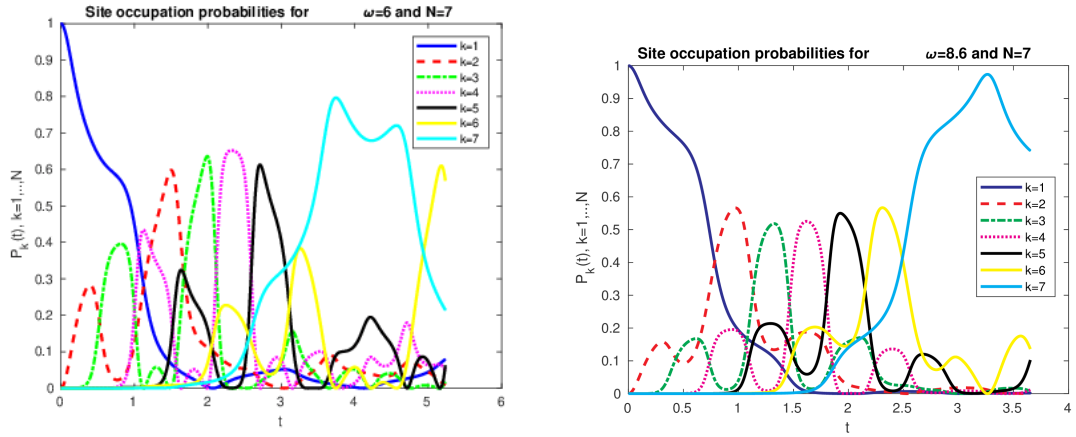


Figure 4.13: Site occupation probabilities $\mathcal{P}_k(t)$ for the two frequencies $\omega_v = 6$ and $\omega_v = 8.6$, and for $m = 7$, $N = 7$.

What can be observed from the series of Figures 4.12-4.14 is firstly that for a fixed mode ($m = 7$ for ex.) not all frequencies of the underlying motion are equally efficient for the excitation transfer from one end to the other end of the spin-chain. Indeed, for $\omega_v \equiv 3$ (left of Fig. 4.12) one remarks that the excitation is trapped between the first three spins, and does not reach the last spin. On Figures 4.12 (right) and 4.13 (left) we observe that the evolution of the excitation is that of a dispersed wave, which is not fully attaining the end point, but is somehow distributed over the whole chain. Finally it seems that starting from one particular frequency ($\omega_\star \approx 8.6$ in the breathing-case $m = 7$) the excitation is quasi fully transferred, frequency which corresponds again to a synchronization as for the chain of two spins (see right of Fig. 4.13 as well as Fig. 4.14).

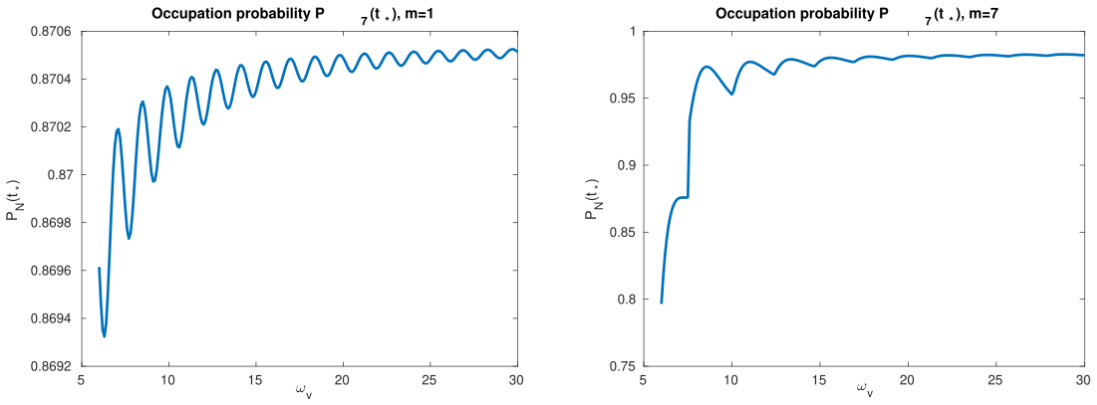


Figure 4.14: Site occupation probability $\mathcal{P}_7(t)$ as a function of the mech. frequency ω_v and for mode $m = 1$ (left) and $m = 7$ (right).

Secondly, we observe that there is a difference in the efficiency when comparing different modes of the mechanical oscillations, the "breathing" mode $m = 7$ being the most efficient one, as observed in Fig. 4.14, where for $m = 1$ one gets $\mathcal{P}_7(t_\sharp) \approx 0.87$ at $t_\sharp \approx 4.45$ and for $m = 7$, $\mathcal{P}_7(t_\sharp) \approx 0.983$ at $t_\sharp \approx 3.45$.
Finally a moving configuration surpasses the maximal static configuration (with $\lambda_{max} = \frac{1}{(1-2a)^3}$, $\mathcal{P}_7(t_\sharp) \approx 0.882$ at $t_\sharp \approx 0.56$) in the sense that the occupation probability $\mathcal{P}_7(t)$ attains values closer to one for the dynamical, synchronized configuration. Remark however that the fastest transfer, even if not complete, occurs for the maximal static coupling strength λ_{max}. Figure 4.15 presents a plot of the occupation probability for constant λ_{avg}, which is simply a time-dilatation or rescaling of the identical probabilities for λ_{max} and compares this plot with a driven configuration.

Some explanations for all these observed phenomena are the following:

- the quantum coherent excitation transfer allows to transfer the **entire** excitation (if there is a synchronization) from one site to the next one, fact which is not possible in a classical excitation transfer (via hopping);

- a modulation of the coupling strength can extend the effective time during which the

excitation is localized close to the next site, as compared to the static configuration, and in this way permits a more efficient excitation transfer.

The fact that a well-orchestrated time-dependent coupling strength permits to enhance the excitation transfer as compared to a uniform coupling with strength λ_{max}, is a pure quantum mechanical effect. This provides a first evidence that biological systems (handling at room temperature) take advantage of non-trivial quantum mechanical effects in order to render its underlying processes efficient.

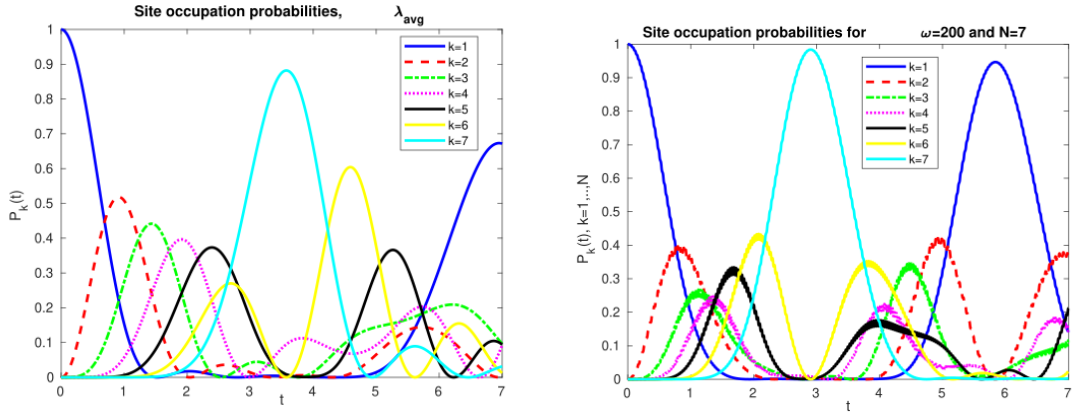


Figure 4.15: Site occupation probabilities $\mathcal{P}_k(t)$ for $N = 7$ and a constant coupling strength λ_{avg} (left) as well as a very high frequency $\omega_v = 200$ in the mode $m = 7$.

4.4 Conclusions and prospects

This model aimed to explore the role of vibrations in excitation energy transfer (EET) within photosynthetic complexes. We focused on examining the impact of unavoidable classical vibrations within a molecular chain on the quantum excitation energy transfer. Unlike a previous study [73] in which a fully quantum model was applied, a hybrid quantum-classical model has been used here to represent the EET. Additionally, molecular motion is considered herein as a coordinated driving force for the excitation transfer, rather than just a disturbance source. Given the small number of molecules, about $N \sim 7$, participating in excitation transfer in photosynthesis complexes, a detailed microscopic mathematical description is utilized. Conversely, for larger spin-chains, it is necessary to adopt the Master-equation formalism because the numerical computations become impractical for chains exceeding $N \sim 14$.
The numerical simulations conducted here revealed that the pigment molecules within the photosynthesis complex engage in a coordinated movement to enhance performance. The precise synchronization between the vibrational movement of the molecular chain and the wave like quantum excitation transfer effectively elevates the efficiency of the transfer beyond static configurations. This motion induced enhancement in excitation transfer is a true quantum hallmark of natural biological processes.

Interestingly, it has been observed that the coupling strength $\lambda(t)$ is integrated into the computation of the site occupation probability. Hence, minor fluctuations in these coupling coefficients, potentially caused by environmental noise, are less likely to have severe impacts compared to a static coupling situation. This aspect will be explored in future research. Another topic for future studies is to expand this model or these concepts to broader, multi-dimensional frameworks, working with quantum networks. The existence of multiple pathways between the photon-acceptor and the photon-receiver, which could coherently interact, might further bolster the excitation energy transfer.

Chapter 5

Perspectives

5.1 Numerical simulations

The development of quantum hybrid models involving increasingly complex structures and the need to obtain even numerical solutions as geometric properties vary lead to the necessity of having modern and versatile simulation tools. The idea, therefore, is not to use traditional numerical models but to employ systems where knowledge of the physical model can facilitate the reconstruction of a solution or at least its fundamental characteristics. The physics-informed neural networks (PINNs) have been of great help in investigating partial differential equations, including quantum PDEs like the Schrödinger equation, since they embody the governing physical laws into the training process as constraints, hence the interest in such a data-efficient approach. In fact, PINNs rely on the equations themselves and on boundary, and initial conditions. PINNs are particularly applicable to high-dimensional problems, which are standard in quantum many-body systems where standard numerical methods suffer from the curse of dimensionality, and have been applied to such problems as quantum wells and tunneling phenomena [81]. Dealing with irregular domains and complex geometries is another strong point of PINNs, naturally appearing when considering quantum systems with complicated potentials or hybrid geometries [82]. This approach enables the studies to even include quantum constraints, such as unitarity and conservation laws, into a loss function together with prescribed boundary conditions, in such a way that the solutions they are looking for will be constrained to respect the basic axioms of quantum mechanics, as already illustrated in many independent investigations considering time-dependent Schrödinger equations and solitonic solutions of nonlinear Schrödinger equations. It has some promising results for systems that range from quantum harmonic oscillators to nonlinear Bose-Einstein condensates, and ongoing studies investigate its application in quantum control and quantum simulations; hence, this gives a flexible and numerically efficient framework to solve many quantum PDEs.

5.1.1 What are the PINNs?

The physics-informed neural networks (PINNs) are a class of machine learning technique that incorporate physical laws and domain knowledge into the training process, it can be used to effectively solve problems involving partial differential equations (PDEs) and

other types of nonlinear physical models. PINNs are based on the idea of embedding equations, such as partial differential equations (PDEs), conservation laws, or other physical principles, into the neural network architecture. These equations are typically derived from physics and are part of the problem being solved. The model is trained not only to minimize the error in predicting outputs but also to satisfy these physical laws. Like traditional neural networks, PINNs use a neural network architecture to approximate solutions to a problem. They learn a mapping between inputs (such as spatial and temporal coordinates) and outputs (such as temperature, velocity, or pressure), but the training process is constrained by the physics-based constraints. More precisely, PINNs approximate PDE solutions by traing a neural network to minimize a loss function. It typically consists of two parts; the first part is the data-driven loss, this term ensures that the neural network approximates the actual data (observed values or boundary conditions), the second part is the physics-based loss, this term penalizes the network when the solution violates the underlying physical laws (e.g., the governing PDEs).

This ensures that the predictions adhere to the physical constraints. PINNs are deep learning networks that, given an input point in the integration domain, produce an estimated solution in that point of a differential equation after training. The network is trained using optimization algorithms like gradient descent. The loss function, which includes both the data-driven and physics-based components, is minimized during training, ensuring that the model not only fits the data but also satisfies the physical laws governing the system. The basic concept behind PINN training is that it can be thought of as an unsupervised strategy that does not require labelled data, such as results from prior simulations or experiments. In summary, Physics-Informed Neural Networks (PINNs) offer a powerful tool for solving real-world problems where both data and physical laws must be taken into account. They have the potential to revolutionize computational modeling by bridging the gap between traditional physics-based simulations and modern machine learning approaches. Let us consider the following Cauchy problem

$$\begin{cases} u_t(t,x) + \mathcal{N}[u(t,x)] = 0 & \text{in } [0,T] \times \Omega \\ u(0,x) = \overline{u}(x) & \text{on } \Omega \\ u(t,x) = \overline{u}(t,x) & \text{on } [0,T] \times \partial\Omega \end{cases}$$

In the PINN methodology, $u(t,x)$ is computationally predicted by NN, parametrized by a set of parameters θ. In such a background, the NN must learn to approximate the differential equations through finding θ by minimizing a loss function that depends on the differential equation, the boundary conditions, and eventually some known data, each of them adequately weighted. Hence, in each epoch (see Figure 5.1), the approximating function is defined

$$u^\theta(x) = C_k \circ \alpha \circ \cdots \circ \alpha \circ C_1(x)$$

where $C_j(x_j) = \omega_j \cdot x_j + b_j$, α is the activation function and ω_j are the weights for all $j = 1, \ldots, k$. At this point, for given function $u^\theta(t,x)$, we can define the **neural network residual**

$$r^\theta(t,x) = u_t^\theta + \mathcal{N}[u^\theta].$$

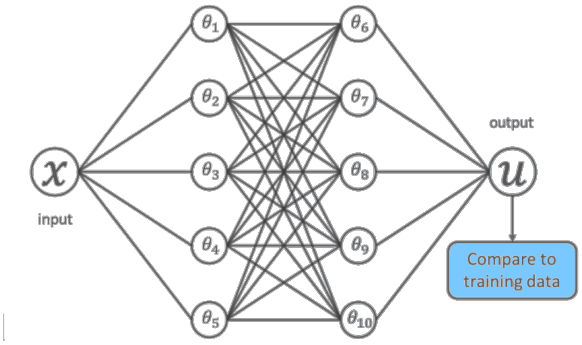


Figure 5.1: A single epoch in the PINN

The PINNs approximate PDE solutions by training a neural network to minimize a following loss functions:

$$\text{Loss}_r(t,x,\theta) = \frac{1}{N_r}\sum_{i=1}^{N_r}|r^\theta(t_i,x_i)|^2;$$

$$\text{Loss}_b(t,x,\theta) = \frac{1}{N_b}\sum_{j=1}^{N_b}|u^\theta(t_j,x_j) - \overline{u}(t_j,x_j)|^2;$$

$$\text{Loss}_0(t,x,\theta) = \frac{1}{N_0}\sum_{k=1}^{N_r}|u^\theta(0,x_k) - \overline{u}(x_k)|^2.$$

Summing up, the neural network will be trained to minimize this loss functions, ensuring that the learned solution obeys the given equation as closely as possible. The network, first of all, takes inputs (variables) and processes them to produce outputs (the field u), which depend on the network's parameters θ. The derivative of the output field u is then calculated using the given equations. It also checks the boundary and initial conditions, if not already incorporated in the network, and evaluates any available labeled data. Finally, the optimizer adjusts the network's parameters θ to minimize the loss, based on a specific learning rate (see [80] for more detail).

5.1.2 Applying PINNs to the Schrödinger Equation

When applying Physics-Informed Neural Networks (PINN) to solve the Schrödinger equation, the main idea is to train a neural network that learns a solution to the equation, while simultaneously making sure that the learned solution follows the governing principles of quantum mechanics, as described by the Schrödinger equation. The time-dependent Schrödinger equation in one dimension is given by

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \widehat{H}\psi(x,t)$$

where:

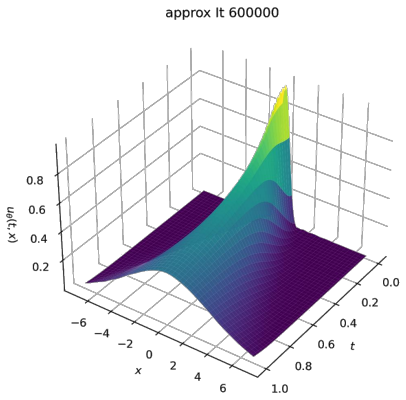


Figure 5.2: $\lambda = 0.7$

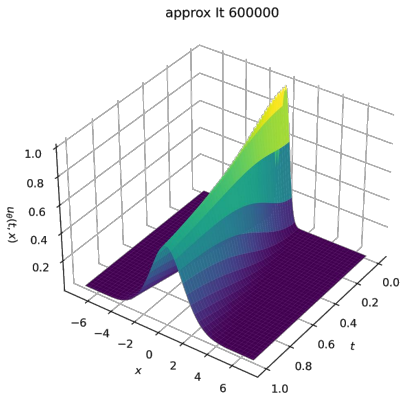


Figure 5.3: $\lambda = 0.3$

1. $\psi(x,t)$ is the wave function of the quantum system, which contains all the information about the system's state;

2. $\widehat{H}$ is the Hamiltonian operator, typically expressed as:

$$\widehat{H} = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{5.1}$$

   where $\hbar$ is the reduced Planck's constant, m is the particle's mass, and $V(x)$ is the potential energy function.

A neural network is used to approximate the wave function $\psi(x,t)$. The inputs to the neural network would typically be the spatial coordinate x and time t, and the output would be the predicted value of the function $\psi(x,t)$. If there are boundary or initial conditions (e.g., the value of the wave function at certain points or times), these can be incorporated into the loss function. For instance, you might have $\psi(x,0) = \psi_0(x)$, where $\psi_0(x)$ is the initial condition. An example problem is the nonlinear Schrödinger equations on line:

$$\begin{cases} i\psi_t + \psi_{xx} + \lambda\,|\psi|^2\psi = 0 & \text{in } [0,1]\times\mathbb{R} \\ \psi(0,x) = e^{-\pi x^2} & \text{on } \mathbb{R} \\ \lim\limits_{x\to\pm\infty}\psi(t,x) = 0 & \text{for any } t\in[0,1]. \end{cases}$$

The plots of the solution are presented in Fig. 5.2 and in Fig. 5.3. In addition the loss function ensures that the neural network's solution satisfies the Schrödinger equation. To enforce the Schrödinger equation the network will compute the partial derivatives of $\psi(x,t)$ with respect to time and space. The loss function will penalize any discrepancy between the network's prediction of the left-hand side of the (5.1) and the right-hand side, which involves both the spatial second derivative $\frac{\partial^2}{\partial x^2}\psi(x,t)$ and the potential term $V(x)$.

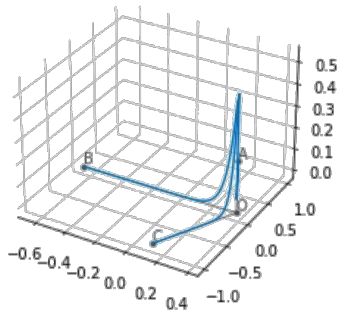


Figure 5.4: t=0.1

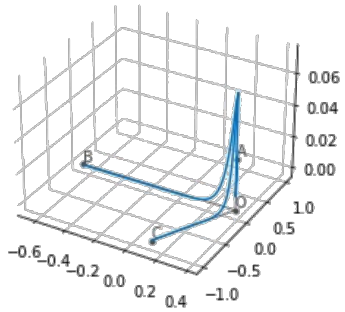


Figure 5.5: t=0.7

5.1.3 The solution of th NLSE on Star Graph using PINN

Definition 5.1.1 (Star graph)**.** A **Star graph** G is a set made up of edges joined together at the same vertex.

We focus on the case of a star graph with 3 edges. Let us indicate:

- the set of edges of the graph with $E = \{e_j\}$;
- the set of vertices of the graph with $V = \{v_k\}$.

To assign Ψ on G means to assign its edge components $\{\psi_e\}_{e\in E}$ with $\psi_e : I_e \to \mathbb{C}$. Now we assume that $n = 1$, $\alpha = 3$, $\lambda = -1$, and to obtain a standing wave on each edges we have to consider the non linear Schrödinger equation with this initial and boundary conditions:

$$\begin{cases} i\psi_t + \psi_{xx} + \psi|\psi|^2 = 0 & \text{in } [0,1]\times\mathbb{R} \\ \psi(0,x) = e^{i\frac{\pi}{4}}\sqrt{2(1-\tanh^2(x+1))} & \text{on } \mathbb{R} \\ \lim\limits_{x\to\pm\infty}\psi(t,x) = 0 & \text{for any } t\in[0,1]. \end{cases}$$

We have to repeat this for each edge of the graph. Setting $\psi = u + iv$, we arrive to a system of coupled equations. The plots of the real part of the solution at different times are presented in Fig. 5.4 and Fig. 5.5. Once the PINN has been trained, it can be used to solve for the wave function $\psi(x,t)$ at any point in space and time, even in regions where no data is available, but the physics (Schrödinger equation) remains valid. This approach is useful for simulating quantum systems where the potential $V(x)$ may be complex, or when traditional methods for solving the Schrödinger equation (e.g., finite difference or finite element methods) are computationally expensive or difficult to apply. By using PINNs to solve the Schrödinger equation, we leverage both the flexibility and power of deep learning while ensuring the solution adheres to fundamental physical laws. This approach can be particularly useful for solving complex quantum mechanical systems where traditional numerical methods may be challenging or impractical.

PINNs are particularly valuable in this context of metric quantum graphs and quantum hybrids because these problems often involve complex boundary conditions at the

vertices, where continuity and flux conservation must be maintained. Traditional numerical methods can struggle with the intricate geometry and nonlinearity of quantum models, especially as the manifolds's complexity increases. PINNs, however, can integrate these boundary conditions directly into their loss functions, ensuring that solutions naturally respect the graph's topology and the physical constraints imposed by quantum mechanics [78, 82].

The main idea in this direction is to adapt PINNs to explore the impact of the geometry of hybrids on quantum dynamics, eigenvalue distributions, and stationary states. PINNs have been shown to excel in solving both forward problems, such as computing wave functions or eigenstates, and inverse problems, such as reconstructing potential functions or graph configurations from observed data [81].

Moreover recent studies have demonstrated the effectiveness of PINNs in modeling quantum transport phenomena on graphs, solving the Schrödinger equation on graphs, and simulating nonlinear dynamics, such as solitonic behavior [79]. These applications highlight the versatility of PINNs in bridging analytical and numerical methods, offering a modern and efficient framework for tackling challenges in the study of quantum hybrids.

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