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Point Interactions in Quantum Mechanics and Acoustics

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Contents

Introduction

An approach based on the construction and the analysis of simple mathematical models is used in this thesis to investigate two kinds of problems in classical theoretical physics: the appearing of classical behavior in quantum systems and the dynamics of fields together with their own sources in acoustics.
The former is a typical problem associated to the investigation of the frontier between theories describing phenomena on different scales.
Actually there is no example of a completely successful reduction from a theory on a higher hierarchic level to one on a lower level. The Boltzmann attempt of explanation of thermodynamics laws in mechanical terms is a paradigmatic example of the enormous difficulties of such reduction programs.
The theory of decoherence gives an explanation of the disappearing of quantum features in terms of interaction of subsystems with the environment.
The loss of quantum coherence in a subsystem is a trivial consequence of the interaction and of the process of reduction of the density matrix. Our efforts are addressed to analyze the manner and the characteristic times with which this happens.
The search for a complete theory of the field with its point sources is a well known topic in electromagnetism. We analyze the analogous subject in acoustics.
Our investigations are in the same line with what was done in the framework of the decoherence program. One expects that in a system consisting of a subsystem with discrete spectrum (the mechanical oscillators) and another subsystem with continuous spectrum (the acoustic field) the energy diffuses all on the continuous spectrum. Our aim is to give an explicit example of system for which the expected result can be proved and to obtain some estimates for the characteristic times of the diffusion of energy.
The approach followed and the type of problems analyzed makes clear our need to have suitable mathematical tools. Since they generate non-trivial but explicitly computable dynamics point interactions have revealed very useful both in the analysis of quantum mechanical and acoustical systems.
The structure of the thesis is the following.
In the first part we analyze two applications of point interactions in the framework of the decoherence program.
In a brief introduction we discuss the reasons that have led to the formulation of the program, basic ideas laying underneath, its relevance in theoretical physics and some practical applications of the results related to the decoherence theory.
Chapter 1 is devoted to a brief historical and mathematical introduction to point perturbations of the Laplacian. A detailed description of the way the theory of

self-adjoint extensions of symmetric operators is used to obtain all the singular perturbations of the Laplacian in one and three dimensions is given.
In chapter 2 point perturbations of the Laplacian in three dimensions are used to study the evolution of a system consisting of two particles interacting via a repulsive point potential and undergoing a single scattering event. The estimates obtained for the asymptotic dynamics in the limit of small mass ratio are used to evaluate the effects of decoherence induced by the interaction.
In the last chapter of part I we analyze the dynamics of a system made up of a quantum particle and one localized spin interacting via a point potential that depends on the state of the spin. We discuss the applications of our model to estimate the loss of quantum coherence due to the interaction.
The second part of the thesis begins with a short introduction to the motivations that have led us to use point perturbations to study a problem of sources interacting with their own field in acoustics.
In the following chapter we introduce our model and express the results obtained in a one dimensional setting for a finite and infinite number of sources and in the continuum limit.
Few pages in which we summarize our results and discuss the future developments of our research conclude the thesis.

Part I

Point Interactions in Quantum Mechanics

Point interactions were introduced in quantum mechanics as point limits of short range potentials in the Schrödinger equation. In order to understand the structure of nuclei it appeared conceivable to analyze general features about interactions with a range much smaller then the atomic size. The zero range limit was justified by the lack of a physically relevant minimal length and as a tool to investigate the low-interaction-energy regime. Only recently a complete characterization of the family of Hamiltonians with point interactions was made available. The quantum dynamics they generate is at the same time non trivial and explicitly computable.

In the following we will discuss two applications of such Hamiltonians in the framework of the decoherence program.

Physical models are always realized to work on a suitable scale (of time, length, energy or number of elements). An important and non trivial task is to define the range of applicability of physical models and to investigate the hierarchic structure of different theories. A fundamental example is the study of the borderline between quantum and classical mechanics.

Some of the most peculiar and counterintuitive features of quantum theory are consequences of the superposition principle. While results of experiments on "microscopic" systems support the validity of the superposition principle every day experience leads to the conclusion that it does not hold for "macroscopic" objects. A popular wisdom suggests that what discriminate a classical system from a quantum one is the large number of components.

It is a puzzling problem to understand how large a "large number" should be. In fact experiments on Bose-Einstein condensates show that systems consisting of several thousands of atoms behave in a quantum fashion for times of the order of milliseconds. On the other side the binding in a molecule, composed of few atoms, is fairly well described by using rods and strings. It is evident that the number of components cannot be the only parameter to define which systems are classical. A clearer understanding of the physical mechanism that leads a quantum object to behave as a classical one is needed.

Schrödinger equation has revealed an extraordinary tool to describe the behavior of a great number of systems on the atomic scale. On the other hand the "classical behavior" of a "macroscopic" object was never derived starting with a quantum mechanical description of its "microscopic" components.

The decoherence program attempts, and partially succeeds, in shading some light on the problem of the quantum origins of classical behavior. The program is based on the idea that even a weak interaction of the subsystem with its environment causes a diffusion of quantum correlations towards the whole system leading to a suppression of interference effects in the subsystem.

This idea dates back to the origins of Quantum Mechanics (see e.g. [33]), but the modern formulation of the decoherence program appeared in the early 1970s in the papers of H.D. Zeh ([56], [57]). The work on the program continued in the following years in particular with W.H. Zurek ([58], [59], [60]). For a recent review on the decoherence program see [61] and [44]. In recent years interest in decoherence has gone beyond the subject of the foundations of quantum mechanics. Experiments in mesoscopic physics [34] and developments on quantum computing [54] are only two examples of fields of application of the results connected with the theory of decoherence.

In the original scheme of the decoherence program physical systems are arranged in three subsystems conventionally referred to as observable, apparatus

and environment. This is basically related to technical reasons connected with Schmidt's theorem (see e.g. [44]). Since we are not going to investigate the problem of the preferred basis we will not make use of such decomposition.
We will consider systems made up of only two quantum subsystems $\mathcal{A}$ and $\mathcal{B}$. The state of the system is a vector in the product Hilbert space

$$\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b \tag{1}$$

and its dynamics is generated by the Hamiltonian

$$H = H_a + H_b + H^{int} \tag{2}$$

where H_a and H_b describe the "free" evolution of subsystem $\mathcal{A}$ and $\mathcal{B}$ respectively while H^{int} determines interaction.
At an intuitive level the mechanism of decoherence is very simple: interaction induces entanglement between subsystems; ignorance about the subsystem $\mathcal{B}$ corresponds to take the trace over $\mathcal{H}_b$ and this procedure partially cancels correlations making the reduced density matrix in $\mathcal{H}_a$ a statistical mixture, even when the initial state of the system is a pure state.
Although there are opinions not supporting the relevance of the decoherence theory as a solution of the measurement problem it is generally accepted that this mechanism plays an important role in explaining the transition from quantum to classical.
We will avoid general questions inside the debate on the foundations of quantum mechanics. Our aim, in line with many other works in literature, is to provide concrete examples of systems for which one can show that decoherence leads an initially quantum subsystem to appear more classical.
In the following the subsystem $\mathcal{A}$ will be a quantum particle. The subsystem $\mathcal{B}$, on which we take the trace, represents the environment (or the measurement apparatus). In principle subsystem $\mathcal{B}$ should be "larger" (made up of a greater number of elements) of $\mathcal{A}$, so that the trace over $\mathcal{B}$ will correspond to a high loss of information. On the other hand the energy exchange should be weak enough to left almost unchanged the dynamics of subsystem $\mathcal{A}$.
We study the evolution of the whole system generated by the Schrödinger equation to detect the entanglement dynamically induced. This allows us to investigate the effects of tracing out the environment. To reach our goal we make use of the highly computable dynamics generated by point Hamiltonians.
The entanglement induced by an event of scattering between two particles is analyzed in the limit of small mass ratio. In the system the "light" particle is intended to represent the environment. While the "heavy" particle proceeds substantially free the "light" particle is "instantly" sent in its scattering state. The attenuation of interference fringes observed in the evolution of an initial state of the heavy particle made up of a superposition of head-on colliding wave packets is a clear sign of decoherence. A better model of environment should be realized with N "light" particles. For a generic smooth potential the expected result that the decoherence effects exponentially grow with N has been proved in a recent work by R. Adami, R. Figari, D. Finco and S. Teta (preprint in preparation).
In the other system analyzed the environment is made up of a lattice of spins. The idea is to realize a model for a measurement apparatus recalling a Wilson chamber in which the atoms ionized by the passage of the particle are replaced

by spins. We were able to define spin dependent point interactions and to analyze the entanglement between a particle and a single spin.
The following step consists in generalizing the Hamiltonian to the case of N spins. A realistic model of Wilson chamber should be realized by interacting spins initially in a metastable state. It is commonly believed that this will produce an enhancement of the decoherence effects.

Chapter 1

Singular Perturbations of the Laplacian

In 1930s there was great interest in modelling the interaction between nucleons. The structure of the nucleus and the early experiments of scattering of neutrons by heavy nuclei suggested that interaction between nucleons should have been with very short range. In those years the idea of a potential with zero range was proposed.
If exists such potential should represent the simplest model of potential with very short range. A particle moving in a potential supported by a point should propagate as a free particle everywhere except in the point in which the potential is placed.
This kind of potential exists in one, two and three dimensions and represents a non trivial but completely solvable limit model of potential with very short range.
Formally the Hamiltonian describing a free particle everywhere except that in the point y should be (in natural units, $\hbar^2/2m = 1$)

$$\text{“}H_\alpha = -\Delta + \alpha\delta_y\text{”} \tag{1.1}$$

where Δ is the Laplacian, α is a real constant and δ_y is the Dirac delta centered in the point y. If the point y is not in the support of the wave function, the particle has only kinetic energy else there is also a term of potential energy.
Inverted commas indicate that formula (1.1) is only a formal writing and thirty years was needed from its introduction in one dimension to a satisfying mathematical formulation as self-adjoint operator in three dimensions.
This chapter is devoted to clarify the meaning of the Hamiltonian (1.1).

1.1 A brief history of H_α

Historically the first relevant model in quantum mechanics based on point interactions dates back to 1931 when the article of Kronig and Penney [31] was published. Kronig and Penney studied the motion of electrons in solids. They considered a one dimensional setting in which ions are fixed and placed on the sites of a regular lattice. Every ion is supposed to produce a zero range potential for the electrons in the conduction band that are considered non interacting, thus the Hamiltonian for one electron in the conduction band is

$$H^{KP} = -\frac{d^2}{dx^2} + \sum_j \alpha_j \delta_{y_j} \tag{1.2}$$

where j runs over the points of the lattice, α_j are real constants and δ_{y_j} is the Dirac delta centered in y_j. In (1.2) we omitted inverted commas because in dimension one, and only in dimension one, formula (1.1) represents a well defined operator. It is possible to obtain the domain of H^{KP} in few simple steps, consider the equation

$$i\frac{d}{dt}\psi = H^{KP}\psi = -\frac{d^2}{dx^2}\psi + \sum_j \alpha_j\, \delta_{y_j}\psi \tag{1.3}$$

by integrating in x from $y_j - \varepsilon$ and $y_j + \varepsilon$ and taking the limit $\varepsilon \to 0$, one obtains

$$\psi'(y_j^+) - \psi'(y_j^-) = \alpha_j \psi(y_j)\,. \tag{1.4}$$

Thus in one dimension $-\Delta + \sum_j \alpha_j \delta_{y_j}$ corresponds to the Laplacian with domain whose elements are continuous functions with first derivative discontinuous in y_j and satisfying boundary condition (1.4). In the following we will give a more precise mathematical definition of the Hamiltonian H^{KP}. However the essence of the operator H^{KP} is completely kept in the boundary condition (1.4), which is all that one needs to study in detail the spectrum of H^{KP}. This is what Kronig and Penney did, in the special case of a periodic lattice with $\alpha_j = \alpha$, obtaining the band structure of metals.

In two and three dimensions it is not possible to derive the structure of the domain of H_α by simple integration as was done in one dimension. Because of the singularities that characterize the Green's functions of the free Schrödinger operator in two and three dimensions also perturbation theory fails when applied to the operator H_α, it is easy to verify that the series expansion of resolvent $(H_\alpha - z)^{-1}$ with $z \in \mathbb{C}\backslash\mathbb{R}$, diverges already at the second order in dimension greater than one.

In spite of these difficulties since 1930s physicists worked to understand if Hamiltonian (1.1) could have made sense in dimension three. This topic was particularly interesting in nuclear physics, where was clear that a zero range potential should have represented a perfect model of potential between nucleons and in problems of scattering with slow neutrons. Bethe-Peierls [12] and Thomas [53] started to study Hamiltonian (1.1) in dimension three. They obtained an approximation of H_α by means of local, scaled short-range potentials realizing that a renormalization of the coupling constant was necessary. Similar results were obtained, almost at the same time, by Fermi [24] in his work about the motion of neutrons in hydrogeneous substances where he introduced for the first time the Fermi pseudo-potentials that can be identified with point interactions, for this reason sometimes, usually in nuclear physics, point interactions are referred to as Fermi pseudo-potentials.

For the first precise mathematical definition of Hamiltonian (1.1) in dimension three we have to wait until the publishing of the work by Berezin and Faddeev [11] in 1961. For the first time H_α was written as a self-adjoint operator derived by using Krein's theory of self-adjoint extensions.

A simple definition of H_α in three dimensions is

$$D(H_\alpha^{3d}) = \Big\{ \psi \in L^2(\mathbb{R}^3) : \psi(x) = \psi^0(x) + \frac{q}{4\pi|x-y|};\ \psi^0 \in H^2_{loc}(\mathbb{R}^3), \\ \nabla\psi^0 \in L^2(\mathbb{R}^3),\ \Delta\psi^0 \in L^2(\mathbb{R}^3),\ q = \frac{\psi^0(y)}{\alpha} \Big\} \tag{1.5}$$

$$H_\alpha^{3d}\psi = -\Delta\psi^0 \tag{1.6}$$

where $H^2_{loc}(\mathbb{R}^3)$ indicates the homogeneous Sobolev space of locally square-integrable functions with their first and second (distributional) derivative. Notice that functions in $D(H_\alpha^{3d})$ may have a singularity in y of order $|x-y|^{-1}$, hence does not make sense to apply the distribution δ_y on $D(H_\alpha^{3d})$.
The operator defined by (1.5) and (1.6) matches up with the point Hamiltonian formally written in (1.1) in the sense that if $y \notin \text{supp}[\psi^0]$ functions ψ and ψ^0 coincide and H_α^{3d} acts on ψ as $-\Delta$.
At the present time operators of the class of H_α are well known and completely classified, the reader interested can refer to the "Bible" [9] and references therein. Examples of recent applications of point Hamiltonians in modern mathematical physics concern time dependent and non-linear problems (see e.g. [18], [19], [4], [1], [2]).
In the following two sections we discuss the structure and the characterization of all the point perturbations of the Laplacian in one and three dimensions by using the theory of self-adjoint extensions briefly discussed in appendix A.

1.2 Singular perturbations of $-\Delta$ in one dimension

We call *singular perturbations of operator* $-\Delta$ *in the point* y all the self-adjoint operators which coincide with the Laplacian everywhere except that in the point y. All the singular perturbations of the Laplacian can be derived by using the theory of self-adjoint extensions described in appendix A.
Hamiltonian H_α is a singular perturbation of $-\Delta$ and can be derived by extending several symmetric operators. Since in dimension one H_α is not the only singular perturbation of $-\Delta$ we will follow a very general construction to obtain all the singular perturbations of the Laplacian, afterwards we will analyze with more detail the one corresponding to the operator (1.1).
Consider the symmetric (closable) operator

$$D(H_0) = C_0^\infty(\mathbb{R}\backslash\{y\}) \qquad y \in \mathbb{R} \tag{1.7}$$

$$H_0\psi = -\frac{d^2}{dx^2}\psi \qquad \psi \in D(H_0). \tag{1.8}$$

Functions ϕ^z satisfying the equation

$$(\phi^z, H_0\psi) = (z\phi^z, \psi) \qquad \phi^z \in L^2(\mathbb{R}),\ \psi \in D(H_0),\ z \in \mathbb{C}\backslash\mathbb{R}\,, \tag{1.9}$$

if exist, are eigenfunctions of H_0^* relative to the eigenvalue z, where * indicates the adjoint. In fact (1.9) is equivalent to

$$H_0^*\phi^z = z\phi^z \qquad \phi^z \in D(H_0^*),\ z \in \mathbb{C}\backslash\mathbb{R}\,. \tag{1.10}$$

A solution of equation (1.9) is

$$G^z(x-y) = -\frac{e^{i\sqrt{z}|x-y|}}{2i\sqrt{z}} \qquad z\in\mathbb{C}\backslash\mathbb{R}^+,\ \mathrm{Im}\,(\sqrt{z})>0 \tag{1.11}$$

In fact $G^z \in L^2(\mathbb{R})$ and satisfies, in the sense of distributions,

$$\left(-\frac{d^2}{dx^2}-z\right)G^z=\delta_y \qquad z\in\mathbb{C}\backslash\mathbb{R}^+\,, \tag{1.12}$$

where δ_y is the Dirac delta centered in y. It is easily seen that

$$(G^z)'(x-y) = -\frac{\mathrm{sgn}(x-y)}{2}e^{i\sqrt{z}|x-y|} \qquad z\in\mathbb{C}\backslash\mathbb{R}^+,\ \mathrm{Im}\,(\sqrt{z})>0 \tag{1.13}$$

where the apex indicates the derivative with respect to x, is another independent solution of equation (1.9) and there are not other solutions of (1.9) independent from G^z and $(G^z)'$. Then $\{G^i,(G^i)'\}$ and $\{G^{-i},(G^{-i})'\}$ span respectively the deficiency spaces $\mathcal{K}^i$ and $\mathcal{K}^{-i}$ and the deficiency indices of H_0 are $(2,2)$. Two orthonormal basis of $\mathcal{K}^z$ and $\mathcal{K}^{\bar z}$ are $\{g^z,g_1^z\}$ and $\{g^{\bar z},g_1^{\bar z}\}$ respectively where

$$g^z(x-y) = \frac{G^z(x-y)}{\|G^z\|} = i\frac{\sqrt{|z|\mathrm{Im}\,(\sqrt{z})}}{\sqrt{z}}e^{i\sqrt{z}|x-y|} \tag{1.14}$$

$$g_1^z(x-y) = \frac{(G^z)'(x-y)}{\|(G^z)'\|} = -\sqrt{\mathrm{Im}\,(\sqrt{z})}\mathrm{sgn}(x-y)e^{i\sqrt{z}|x-y|} \tag{1.15}$$

$$z\in\mathbb{C}\backslash\mathbb{R}^+,\ \mathrm{Im}\,\sqrt{z}>0\,.$$

Following the von Neumann construction (see appendix A) we have that if U is a unitary application from $\mathcal{K}^i$ to $\mathcal{K}^{-i}$, operator H^U defined by

$$\begin{aligned} D(H^U) = \Big\{\psi : \psi = \psi_0 + c_1 g^i + c_2 g_1^i + c_1' g^{-i} + c_2' g_1^{-i};\ \psi_0\in D(H_0),\\ c_1,c_2\in\mathbb{C},\ c_m' = \sum_{n=1,2} U_{mn}c_n,\ m=1,2\Big\} \end{aligned} \tag{1.16}$$

$$H^U\psi = H_0\psi_0 + i(c_1 g^i + c_2 g_1^i - c_1' g^{-i} - c_2' g_1^{-i}) \tag{1.17}$$

where U_{mn} is the 2×2 unitary matrix representing the unitary application U in the basis $\{g^i,g_1^i\}$ and $\{g^{-i},g_1^{-i}\}$, is self-adjoint and is an extension of H_0. Moreover all the self-adjoint extensions of H_0 can be written in the form (1.16)-(1.17).

The more general 2×2 unitary matrix can be written as

$$U = \begin{pmatrix} -e^{i\theta}\cos\omega & e^{i(\theta+\rho)}\sin\omega \\ -e^{i(\varphi-\rho)}\sin\omega & -e^{i\varphi}\cos\omega \end{pmatrix} \tag{1.18}$$

$$\omega,\ \theta,\ \varphi,\ \rho\in[0,2\pi)\,.$$

By straightforward calculations one can check that, with this choice of U, functions in $D(H^U)$ satisfy boundary conditions

$$\begin{aligned} \psi(y^+)-\psi(y^-) &= C_1\left(\frac{\psi(y^+)+\psi(y^-)}{2}\right) + C_2\left(\frac{\psi'(y^+)+\psi'(y^-)}{2}\right)\\ \psi'(y^+)-\psi'(y^-) &= C_3\left(\frac{\psi(y^+)+\psi(y^-)}{2}\right) + C_4\left(\frac{\psi'(y^+)+\psi'(y^-)}{2}\right) \end{aligned} \tag{1.19}$$

where C_1, C_2, C_3 and C_4 are complex constants defined by

$$C_1 = -\frac{2\sqrt{2}e^{-i(\rho-\varphi)}\sin\omega}{i(1+e^{i(\theta+\varphi)}) + (e^{i\varphi}-e^{i\theta})\cos\omega} \tag{1.20}$$

$$C_2 = -\frac{(1+i)\sqrt{2}\left(i+e^{i(\theta+\varphi)} - (e^{i\theta}+ie^{i\varphi})\cos\omega\right)}{i(1+e^{i(\theta+\varphi)}) + (e^{i\varphi}-e^{i\theta})\cos\omega} \tag{1.21}$$

$$C_3 = -\frac{(1-i)\sqrt{2}\left(i-e^{i(\theta+\varphi)} - (ie^{i\theta}-e^{i\varphi})\cos\omega\right)}{i(1+e^{i(\theta+\varphi)}) + (e^{i\varphi}-e^{i\theta})\cos\omega} \tag{1.22}$$

$$C_4 = -\frac{2\sqrt{2}e^{i(\rho+\theta)}\sin\omega}{i(1+e^{i(\theta+\varphi)}) + (e^{i\varphi}-e^{i\theta})\cos\omega} \tag{1.23}$$

Constants C_1, C_2, C_3 and C_4 characterize all the singular perturbations of the Laplacian in dimension one via boundary conditions. A different, and well known in literature (see e.g. [17], [7] and [14]), characterization of all the self-adjoint extensions of H_0 reads

$$\begin{aligned} \psi(y^+) &= \eta a\,\psi(y^-) + \eta b\,\psi'(y^-) \\ \psi'(y^+) &= \eta c\,\psi(y^-) + \eta d\,\psi'(y^-) \end{aligned} \tag{1.24}$$

with a, b, c, $d \in \mathbb{R}$, $\eta \in \mathbb{C}$, $ad - bc = 1$ and $|\eta| = 1$. It is possible to show that boundary conditions (1.19) and (1.24) are equivalent, the following relations hold

$$C_1 = -\frac{2(1-\eta^2-\eta(a-d))}{1+\eta^2+\eta(a+d)} \tag{1.25}$$

$$C_2 = \frac{4\eta^2 b}{1+\eta^2+\eta(a+d)} \tag{1.26}$$

$$C_3 = \frac{4\eta^2 c}{1+\eta^2+\eta(a+d)} \tag{1.27}$$

$$C_4 = -\frac{2(1-\eta^2+\eta(a-d))}{1+\eta^2+\eta(a+d)} \tag{1.28}$$

Diagonal unitary matrices ($\omega = 0$ in the formula (1.18)) correspond to a sub-family of extensions of H_0 in which the discontinuity of the function depends only on the value of the left and right limit of the derivative in y ($C_1 = 0$) and the discontinuity of the derivative depends only on the value of the left and right limit of the function in y ($C_4 = 0$). Straightforward calculations show that if $\omega = 0$

$$C_1 = C_4 = 0 \tag{1.29}$$

$$C_2 = \frac{\sqrt{2}(\cos\varphi - \sin\varphi - 1)}{1+\sin\varphi} \tag{1.30}$$

$$C_3 = \frac{\sqrt{2}(\cos\theta + \sin\theta - 1)}{1-\sin\theta} \tag{1.31}$$

Notice that both C_2 and C_3 are real constants and that C_2 depends only on φ while C_3 depends only on θ.

The extension given by $\omega = \theta = \varphi = 0$ corresponds to the operator

$$D(H) = \Big\{ \psi : \psi = \psi_0 + c_1(g^i - g^{-i}) + c_2(g_1^i - g_1^{-i})\,; \\ \psi_0 \in D(H_0),\ c_1, c_2 \in \mathbb{C} \Big\} \tag{1.32}$$

$$H\psi = H_0\psi_0 + i(c_1(g^i + g^{-i}) + c_2(g_1^i + g_1^{-i}))\,. \tag{1.33}$$

Functions in the domain of H are continuous and have continuous derivative in y, from its definition the operator H coincides with the "free" Hamiltonian i.e.

$$D(H) = H^2(\mathbb{R}) \qquad H\psi = -\frac{d^2}{dx^2}\psi \qquad \psi \in D(H)\,. \tag{1.34}$$

Operator $H_\alpha^{1d} = -\Delta + \alpha\delta_y$ is given by $\omega = \varphi = 0$, from boundary conditions (1.19) it is easily seen that

$$D(H_\alpha^{1d}) = \Big\{ \psi \in H^1(\mathbb{R}) \cap H^2(\mathbb{R}\backslash\{y\}) : \\ \psi'(y^+) - \psi'(y^-) = \alpha\psi(y),\ -\infty < \alpha \leq \infty \Big\} \tag{1.35}$$

$$H_\alpha^{1d} = -\frac{d^2}{dx^2}\,. \tag{1.36}$$

Constant α is related to θ by formula (1.31)

$$\alpha = \frac{\sqrt{2}(\cos\theta + \sin\theta - 1)}{1 - \sin\theta} \tag{1.37}$$

Interaction given by Hamiltonian H_α^{1d} is often referred to as δ-interaction.
We indicate with $H_\beta'^{1d}$ the other well known extension of H_0 given by $\omega = \theta = 0$, again boundary conditions (1.19) give

$$D(H_\beta'^{1d}) = \Big\{ \psi \in H^2(\mathbb{R}\backslash\{y\}) :\ \psi'(y^+) = \psi'(y^-), \\ \psi(y^+) - \psi(y^-) = \beta\psi'(y),\ -\infty < \beta \leq \infty \Big\} \tag{1.38}$$

$$H_\beta'^{1d} = -\frac{d^2}{dx^2}\,. \tag{1.39}$$

Constant β is related to φ by formula (1.30)

$$\beta = \frac{\sqrt{2}(\cos\varphi - \sin\varphi - 1)}{1 + \sin\varphi} \tag{1.40}$$

Interaction given by Hamiltonian $H_\beta'^{1d}$ is often referred to as δ'-interaction.
From (1.30), (1.31), (1.37) and (1.40) it is easy to convince ourselves that the subfamily given by $\omega = 0$ corresponds to a point potential given by a δ-interaction plus a δ'-interaction.
Operators H_α^{1d} or $H_\beta'^{1d}$ coincides with H if $\alpha = 0$ or $\beta = 0$ respectively.
Equivalently all the self-adjoint extensions of H_0 can be obtained by using the Krein's formula for the resolvent, such formula allows to evaluate the difference of two resolvents of two different self-adjoint extensions of H_0 (see appendix A).

We indicate with H^Θ the generic self-adjoint extension of H_0, usually it is useful to express the resolvent of H^Θ with respect to the "free" resolvent $(H-z)^{-1}$, formula (A.10) reads

$$(H^\Theta - z)^{-1} = (H-z)^{-1} + \sum_{m,n=1,2} (\Gamma(z))^{-1}_{mn} (\phi^{\bar{z}}_n, \cdot)\phi^z_m \qquad z \in \rho(H^\Theta) \quad (1.41)$$

where functions ϕ^z_m are defined by

$$\phi^z_1(x) = G^z(x-y) \; ; \quad \phi^z_2(x) = (G^z)'(x-y) \qquad z \in \mathbb{C}\backslash\mathbb{R}^+ \quad (1.42)$$

By direct calculation one can check that ϕ^z_m satisfy relation

$$\phi^z_m = \phi^{z_0}_m + (z-z_0)(H-z)^{-1}\phi^{z_0}_m \qquad m=1,2;\; z, z_0 \in \rho(H) \quad (1.43)$$

Matrix $\Gamma(z)$ is defined by

$$\Gamma(z)_{mn} - \Gamma(z')_{mn} = (z'-z)(\phi^{\bar{z}}_n, \phi^{z'}_m) \qquad m,\, n = 1,2;\; z, z' \in \rho(H^\Theta) \quad (1.44)$$

and

$$\Gamma(z)^* = \Gamma(\bar{z}) \qquad z \in \rho(H^\Theta) \quad (1.45)$$

Functions $\Gamma(z)_{mn}$ and ϕ^z_m, are analytic in $z \in \rho(H^\Theta)$, notice that $\rho(H^\Theta) \subseteq \rho(H)$.
Relation (1.44) does not define univocally the matrix $\Gamma(z)$, by direct calculation one can verify that

$$\Gamma(z) = \begin{pmatrix} \frac{1}{2i\sqrt{z}} & 0 \\ 0 & \frac{\sqrt{z}}{2i} \end{pmatrix} + \Theta\,, \quad (1.46)$$

where Θ is a 2×2 arbitrary, constant, Hermitian matrix, satisfies conditions (1.44) and (1.45). Then the resolvent is found by inverting the matrix $\Gamma(z)$ and by formula (1.41). Matrix Θ plays the role of the unitary application U in the von Neumann construction, in fact a 2×2 Hermitian matrix is determined by four real independent parameters. The domain of H^Θ is then given by the range of the resolvent $(H^\Theta - z)^{-1}$.
It is a simple exercise to write down the resolvent of H^{1d}_α. The maximal common part (see appendix A) of H and H^{1d}_α is not H_0 but

$$\ddot{H}_0 = -\frac{d^2}{dx^2}, \quad D(\ddot{H}_0) = \left\{\psi \in H^2(\mathbb{R}) : \psi(y) = 0\right\}\,, \quad (1.47)$$

its adjoint is

$$\ddot{H}^*_0 = -\frac{d^2}{dx^2}, \quad D(\ddot{H}^*_0) = H^2(\mathbb{R}\backslash\{y\}) \cap H^1(\mathbb{R})\,. \quad (1.48)$$

Then the only independent solution of equation

$$(H^*_0 - z)\phi^z = 0 \qquad \phi^z \in L^2(\mathbb{R}),\; z \in \mathbb{C}\backslash\mathbb{R} \quad (1.49)$$

is $G^z(x-y)$. Function

$$\Gamma(z) = \frac{1}{2i\sqrt{z}} - \frac{1}{\alpha} \quad (1.50)$$

with $\alpha \in \mathbb{R}$ satisfies

$$\Gamma(z) - \Gamma(z') = (z' - z)(G^{\bar{z}}, G^{z'}) \qquad z, z' \in \rho(H_\alpha^{1d}) \tag{1.51}$$

and

$$\overline{\Gamma(z)} = \Gamma(\bar{z}) \qquad z \in \rho(H_\alpha^{1d}) \tag{1.52}$$

Then resolvent of H_α^{1d} ca be written as

$$(H_\alpha^{1d} - z)^{-1} = (H - z)^{-1} - \frac{2\alpha\sqrt{z}}{i\alpha + 2\sqrt{z}} (G^{\bar{z}}(\cdot\, - y), \cdot\,) G^z(\cdot\, - y) \qquad z \in \rho(H_\alpha^{1d}) \tag{1.53}$$

and operator H_α^{1d} can be defined as

$$D(H_\alpha^{1d}) = \Big\{ \psi \in L^2(\mathbb{R}) : \psi = \psi^z - \frac{2\alpha\sqrt{z}}{i\alpha + 2\sqrt{z}} \psi^z(y)\, G^z(\cdot\, - y); \; \psi^z \in D(H),\, z \in \rho(H_\alpha^{1d}),\, \mathrm{Im}\sqrt{z} > 0 \Big\} \tag{1.54}$$

$$(H_\alpha^{1d} - z)\psi = (H - z)\psi^z \tag{1.55}$$

Function ψ^z is called regular part of ψ, if $\psi^z(y) = 0$ then $\psi = \psi^z$ and $H_\alpha^{1d}\psi = H\psi$. Starting from formula (1.54) it is easy to verify that functions in $D(H_\alpha^{1d})$ satisfy boundary condition

$$\psi'(y^+) - \psi'(y^-) = \alpha\psi(y) \tag{1.56}$$

As we will see in the following the characterization of the domain $D(H_\alpha^{1d})$ given in formula (1.54), with a regular part plus a term proportional to the value of the regular part in the point y and to the Green's function of the "free" Hamiltonian, is recurrent in the structure of the point perturbations of self-adjoint operators. An exhaustive analysis of all the singular perturbations of $-\Delta$ in one dimension is in [7]. The reader interested will find there the spectrum of H^U for δ and δ'-interactions and the analytic expression of the integral kernel of the propagator in the general case expressed by boundary conditions (1.24).
The generalization to a finite or infinite number of points and the analysis of the band structure obtained with the Kronig and Penney Hamiltonian (1.2) is in [9].

1.3 Singular perturbations of $-\Delta$ in three dimensions

As we stated in section (1.1) in three dimensions it is not easy to obtain an intuitive definition of H_α as it was done in dimension one. In spite of this the procedure to define H_α in three dimensions by using the theory of self-adjoint extensions is substantially identical to the one dimensional case and in some sense more simple.
Consider the operator

$$D(H_0) = C_0^\infty(\mathbb{R}^3 \backslash \{y\}) \qquad y \in \mathbb{R}^3 \tag{1.57}$$

$$H_0\psi = -\Delta\psi \qquad \psi \in D(H_0) \tag{1.58}$$

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$. In three dimensions the only independent solution of equation

$$H_0^*\phi^z = z\phi^z \qquad \phi^z \in D(H_0^*),\ z \in \mathbb{C}\backslash\mathbb{R} \tag{1.59}$$

is

$$G^z(x-y) = \frac{e^{i\sqrt{z}|x-y|}}{4\pi|x-y|} \qquad z \in \mathbb{C}\backslash\mathbb{R},\ \mathrm{Im}\sqrt{z} > 0, \tag{1.60}$$

like in dimension one, G^z satisfies, in the sense of distributions, the equation $(-\Delta - z)G^z = \delta_y$, where δ_y is the three dimensional Dirac delta centered in y, in three dimensions the derivative of G^z is not in $L^2(\mathbb{R}^3)$.
Functions G^i and G^{-i} span the deficiency spaces $\mathcal{K}^i$ and $\mathcal{K}^{-i}$ respectively and the deficiency indices are $(1,1)$. A unitary application between one dimensional spaces is defined by only one real parameter then all the self-adjoint extensions of H_0 are elements of a one real parameter family of self-adjoint operators.
The more general function in $\mathcal{K}^i$ can be written as

$$\phi^i(x) = cG^i(x) \qquad c \in \mathbb{C} \tag{1.61}$$

Being $\|G^i\| = \|G^{-i}\| = (\sqrt{4\pi\sqrt{2}})^{-1}$ a function ϕ^{-i} obtained by ϕ^i via a unitary application U is

$$\phi^{-i} = U\phi^i = -e^{i\theta}cG^{-i} \qquad \theta \in [0, 2\pi) \tag{1.62}$$

Indicating with H^U the self-adjoint extension of H_0 corresponding to the unitary application U, von Neumann formula gives (see appendix A)

$$\begin{aligned} D(H^U) = \Big\{ \psi \in L^2(\mathbb{R}^3) :\ \psi = \psi_0 + c(G^i - e^{i\theta}G^{-i}); \\ \psi_0 \in D(H_0),\ c \in \mathbb{C},\ \theta \in [0, 2\pi) \Big\} \end{aligned} \tag{1.63}$$

$$H^U\psi = H_0\psi_0 + ic(G^i + e^{i\theta}G^{-i}) \tag{1.64}$$

Owing to the presence of the term $c(G^i - e^{i\theta}G^{-i})$ in general functions in $D(H^U)$ are not in $H^2(\mathbb{R}^3)$.
Noticing that

$$\lim_{|x-y|\to 0}(G^i - G^{-i}) = \frac{i\sqrt{i} - \sqrt{-i}}{4\pi} \tag{1.65}$$

one obtains $(G^i - G^{-i}) \in H^2(\mathbb{R}^3)$, then for $\theta = 0$ operator H^U coincides with the "free" Hamiltonian

$$D(H) = H^2(\mathbb{R}^3), \quad H\psi = -\Delta\psi, \qquad \psi \in D(H)\,. \tag{1.66}$$

Function

$$\Gamma(z) = -i\frac{\sqrt{z}}{4\pi} + \alpha \tag{1.67}$$

where α is a real constant, satisfies

$$\Gamma(z) - \Gamma(z') = (z' - z)(G^{\bar{z}}, G^{z'}) \qquad z, z' \in \rho(H_\alpha^{1d}) \tag{1.68}$$

and

$$\overline{\Gamma(z)} = \Gamma(\bar{z}) \tag{1.69}$$

then indicating with H_α^{3d} the self-adjoint extension of H_0 corresponding to α, from Krein's formula one obtains

$$(H_\alpha^{3d}-z)^{-1}=(H-z)^{-1}+\frac{4\pi}{4\pi\alpha-i\sqrt{z}}(G^{\bar z}(\cdot\,-y),\cdot\,)G^z(\cdot\,-y) \tag{1.70}$$

Being $D(H_\alpha^{3d})=\mathrm{Ran}[(H_\alpha^{3d}-z)^{-1}]$ it is easily seen that

$$\begin{aligned} D(H_\alpha^{3d})=\Big\{&\psi\in L^2(\mathbb{R}^3):\,\psi=\psi^z+qG^z(\cdot\,-y);\,\psi^z\in H^2(\mathbb{R}^3),\\ &q=\frac{4\pi\psi^z(y)}{4\pi\alpha-i\sqrt{z}},\,z\in\rho(H_\alpha^{3d}),\mathrm{Im}\sqrt{z}>0,\ -\infty<\alpha\le\infty\Big\}\end{aligned} \tag{1.71}$$

$$(H_\alpha^{3d}-z)\psi=(H-z)\psi^z \tag{1.72}$$

Function $\psi^z(x)$ is called regular part and often constant q is referred to as charge.
Of course formulas (1.71) and (1.72) represent a good prototyped of point interaction in dimension three, in fact if $y\notin\psi^z$ then $\psi=\psi^z$ and $H_\alpha^{3d}\psi=H\psi$.
It is worth to note that constant q does not depend on z, in fact it can be defined as

$$q=\lim_{|x-y|\to 0}4\pi|x-y|\psi(x) \tag{1.73}$$

The operator defined in (1.71)-(1.72) coincides with the one given in (1.5) and (1.6). In fact function

$$\psi^0=\psi(x)-\frac{q}{4\pi|x-y|}=\psi^z(x)+qG^z(x-y)-\frac{q}{4\pi|x-y|} \tag{1.74}$$

satisfies $\psi^0\in H^2_{loc}(\mathbb{R}^3)$, $\nabla\psi^0\in L^2(\mathbb{R}^3)$, $\Delta\psi^0\in L^2(\mathbb{R}^3)$, $\psi^0(y)=\alpha q$ and

$$H_\alpha^{3d}\psi=H\psi^z-z(\psi^z-\psi)= \tag{1.75}$$

$$=-\Delta\left(\psi^0+\frac{q}{4\pi|x-y|}-qG^z\right)+zqG^z=-\Delta\psi^0 \tag{1.76}$$

The real constant α is related to the behaviour of functions in $D(H_\alpha)$ near the point y, in fact

$$\lim_{r\to 0}\frac{\partial r\psi}{\partial r}-4\pi\alpha r\psi=0\qquad \psi\in D(H_\alpha^{3d}) \tag{1.77}$$

where $r=|x-y|$.
The relation between α and θ can be deduced by imposing condition (1.77) on

$$\psi=\psi_0+c(G^i-e^{i\theta}G^{-i})\qquad \psi_0\in D(H_0),\,c\in\mathbb{C} \tag{1.78}$$

one obtains

$$4\pi\alpha=-\frac{\sqrt{2}}{2}\left(1-\frac{\sin\theta}{1-\cos\theta}\right) \tag{1.79}$$

notice that $\alpha\to\infty$ when $\theta\to 0$, then contrarily to the one dimensional case the "free" operator corresponds to $\alpha=\infty$, according to the fact that $-(4\pi\alpha)^{-1}$ represents the scattering length of H_α^{3d}.
Since we will use the operator H_α^{3d} in chapter 2 we state the main results about its spectrum and the integral kernel of propagator $e^{-iH_\alpha^{3d}t}$

Theorem 1.1. *The essential spectrum of* H_α^{3d} *is purely absolutely continuous and*

$$\sigma_{ess}(H_\alpha^{3d}) = \sigma_{ac}(H_\alpha^{3d}) = [0,\infty), \qquad \sigma_{sc}(H_\alpha^{3d}) = \varnothing \tag{1.80}$$

If $\alpha < 0$, H_α^{3d} *has one eigenvalue*

$$\sigma_{pp}(H_\alpha^{3d}) = \{-(4\pi\alpha)^2\} \qquad -\infty < \alpha < 0 \tag{1.81}$$

the corresponding normalized eigenfunction is

$$\phi_0 = \sqrt{2|\alpha|}\frac{e^{4\pi\alpha|x-y|}}{|x-y|} \tag{1.82}$$

If $\alpha \geq 0$, *then* $\sigma_{pp} = \varnothing$.

The proof is based on the analysis of resolvent $(H_\alpha^{3d} - z)^{-1}$, the reader interested can refer to [9].
The integral kernel $U_\alpha^t(x, x')$ of the propagator $e^{-iH_\alpha^{3d}t}$ is obtained by a formal inverse Laplace of the resolvent (see [43], [6], [7])

$$U_\alpha^t(x,x') = U^t(x-x') + \frac{2it}{|x-y||x'-y|}U^t(|x-y|+|x'-y|)+$$
$$+\begin{cases} -\dfrac{8\pi\alpha it}{|x-y||x'-y|}\displaystyle\int_0^\infty e^{-4\pi\alpha u}U^t(u+|x-y|+|x'-y|)du & \alpha>0 \\ 0 & \alpha = 0 \\ 2|\alpha|e^{4\pi i|\alpha|^2 t}\dfrac{e^{-4\pi|\alpha|\,|x-y|}}{|x-y|}\dfrac{e^{-4\pi|\alpha|\,|x'-y|}}{|x'-y|}+ & \\ +\dfrac{8\pi\alpha it}{|x-y||x'-y|}\displaystyle\int_0^\infty e^{4\pi\alpha u}U^t(u-|x-y|-|x'-y|)du & \alpha<0 \end{cases} \tag{1.83}$$

where $U^t(x-x')$ is the integral kernel of the "free" propagator e^{-iHt} in dimension three

$$\left(e^{-iHt}f\right)(x) = \int_{\mathbb{R}^3} U^t(x-x')f(x')dx' = \int_{\mathbb{R}^3}\frac{e^{i\frac{|x-x'|^2}{4t}}}{(4\pi it)^{\frac{3}{2}}}f(x')dx' \tag{1.84}$$

The generalization of the construction to N and infinite points, the approximation by means of local and non local scaled-short range potential and much more is in [9].

Chapter 2

Decoherence Induced by Scattering

We give a rigorous treatment of the asymptotic dynamics of a quantum particle undergoing a single scattering event with a much lighter particle.
A detailed knowledge of such a process is the necessary preliminary step for the formulation of more realistic models for the dynamics of a quantum particle evolving in an environment made up of many light particles. In this perspective this problem was investigated by Joos and Zeh [29] first and by many others ([25], [51], [27], [26], [13] and references therein) successively.
Starting from a dynamical hypothesis about a single scattering event, since then referred to as Joos and Zeh formula, those authors deduced a master equation for the reduced density matrix of the heavy particle, from where they computed the characteristic times of the processes of decoherence and dissipation induced by the interaction.
Joos and Zeh noticed that as a consequence of a small mass ratio two time scales characterize the evolution of the two particles: a slow one relative to the heavy particle and a much faster one relative to the light particle.
In order to specify the details of their idea let us suppose that the state of the two particle system is initially given in a product form of the type $\varphi(R)\chi(r)$ where R and r describe respectively the spatial coordinates of the heavy particle and of the light one. The authors proposed that, in the roughest approximation, the scattering process would be described by the instantaneous transition

$$\varphi(R)\chi(r) \to \varphi(R) \left(S^R\chi\right)(r) \tag{2.1}$$

where S^R is the scattering operator for the light particle corresponding to the heavy one fixed at the position R. The R dependence of the scattering operator indicates that entanglement has taken place in the sense that the state of the scattered light particle keeps track of the position of the heavy one.
Details of the process of entanglement dynamically induced by a single scattering event, outlined above, was analyzed in a series of recent papers ([20], [23] and [3]) for different models of two body interaction. In [23] and [3] the authors gave rigorous estimates of the asymptotic dynamics, in the limit of a small mass ratio, for particles interacting respectively via a point interaction in dimension

one and for a class of smooth potentials in three dimensions. Their results can be considered as a rigorous formulation of the Joos and Zeh formula (2.1).
We give a detailed analysis of the dynamics of a three dimensional system made up of two quantum particles interacting via a repulsive δ-like potential.
All the results presented in this chapter are published in [15].

2.1 The model

In order to define the model we need to introduce some notation and to recall few results concerning scattering theory and wave operators.
We indicate with $H_{\alpha,y}$ the family of self-adjoint perturbations of the free Laplacian in dimension three. The operators $H_{\alpha,y}$ coincide with H_α^{3d} defined in section 1.3.
In order to simplify notation we will use H_α instead of $H_{\alpha,0}$. For $\alpha > 0$ the explicit form of the propagator e^{-itH_α} of H_α (see [43], [6] and [7]) is

$$\begin{aligned} e^{-itH_\alpha}(x,x') =& e^{-itH}(x-x') + \frac{2it}{|x||x'|} e^{-itH}(|x|+|x'|) + \\ & - \frac{8\pi\alpha it}{|x||x'|} \int_0^\infty e^{-4\pi\alpha u} e^{-itH}(|x|+|x'|+u)\, du \end{aligned} \tag{2.2}$$

where H is the "free" Hamiltonian (1.66) and e^{-itH} is the "free" propagator with integral kernel

$$e^{-itH}(x-x') = \frac{e^{i\frac{|x-x'|^2}{4t}}}{(4\pi it)^{\frac{3}{2}}}\,. \tag{2.3}$$

For every $k \in \mathbb{R}^3$ the generalized eigenfunction of $H_{\alpha,y}$ corresponding to the energy $E = |k|^2$ in the continuous spectrum is given in closed form by

$$\Phi_\pm^y(x,k) = e^{ikx} + \frac{e^{iky}}{4\pi\alpha \pm i|k|} \frac{e^{\mp i|k||x-y|}}{|x-y|} \tag{2.4}$$

Using the generalized eigenfunctions $\Phi_\pm^y$ it is possible to define the unitary maps (see e.g. [21]) $\mathcal{F}_\pm^y : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$

$$[\mathcal{F}_\pm^y f](k) = \mathrm{s} - \lim_{R\to\infty} \frac{1}{(2\pi)^{3/2}} \int_{B_R} \overline{\Phi_\pm^y(x,k)} f(x) dx \tag{2.5}$$

where B_R indicates the sphere of radius R in $\mathbb{R}^3$. The wave operators (see e.g. [42] and [46]) for the Hamiltonian $H_{\alpha,y}$

$$\Omega_\pm^y = \mathrm{s} - \lim_{\tau\to\pm\infty} e^{i\tau H_{\alpha,y}} e^{-i\tau H_0} \tag{2.6}$$

are unitary for $\alpha > 0$ and are related to $\mathcal{F}_\pm^y$ by

$$\Omega_\pm^y = (\mathcal{F}_\pm^y)^{-1}\mathcal{F}\,; \quad (\Omega_\pm^y)^{-1} = \mathcal{F}^{-1}\mathcal{F}_\pm^y \tag{2.7}$$

where $\mathcal{F}$ indicates the usual Fourier transform.
Now we have all the ingredients to define our two particle model. The "free" Hamiltonian describing two non interacting particles of mass M and m is the operator

$$D(\mathbf{H}) = H^2(\mathbb{R}^3, dR) \otimes H^2(\mathbb{R}^3, dr) \qquad \mathbf{H} = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2m}\Delta_r\,. \tag{2.8}$$

where R and r are the coordinates relative to the particle of mass M and m respectively while Δ_R and Δ_r indicate the Laplacian with respect to the coordinates R and r. To simplify notation we fix $M = 1$ and $\hbar^2/2 = 1$ and we define $\varepsilon \equiv \frac{m}{M}$.
In the system of coordinates of the center of mass $x \equiv \frac{R+\varepsilon r}{1+\varepsilon}$ and of the relative coordinate $y \equiv r - R$, the Hamiltonian $\mathbf{H}$ reads

$$D(\mathbf{H}) = H^2(\mathbb{R}^3, dx) \otimes H^2(\mathbb{R}^3, dy) \qquad \mathbf{H} = -\frac{1}{\nu}\Delta_x - \frac{1}{\mu}\Delta_y\,. \tag{2.9}$$

where $\nu = (1+\varepsilon)$ is the total mass of the system, $\mu = \frac{\varepsilon}{1+\varepsilon}$ is the reduced mass.
At formal level the operator (2.9) can be written as

$$\mathbf{H} = H^\nu \otimes \mathbb{I} + \mathbb{I} \otimes H^\mu \tag{2.10}$$

where $H^\nu = \nu^{-1}H$ and $H^\mu = \mu^{-1}H$, while $\mathbb{I}$ indicates the identity operator on $L^2(\mathbb{R}^3)$.
The operator

$$\mathbf{H}_\alpha = H^\nu \otimes \mathbb{I} + \mathbb{I} \otimes H^\mu_\alpha \tag{2.11}$$

with $H^\mu_\alpha = (\mu)^{-1}H_\alpha$ is self-adjoint and coincides with $\mathbf{H}$ on functions satisfying the condition $\Psi(R,r)|_{R=r} = 0$. Notice that in (2.11) $H^\mu_\alpha = \mu^{-1}H_\alpha$ suggest that a rescaling of the coupling constant α has been made (compare with the cases of two body potentials [23] and [3]).
We consider the problem

$$i\frac{\partial\Psi(t)}{\partial t} = \mathbf{H}_\alpha\Psi(t) \tag{2.12}$$

$$\Psi(0; R, r) = \varphi(R)\chi(r) \tag{2.13}$$

in the limit of small ε.
Because of the particular initial conditions (2.13) the positions of the two particles are uncorrelated at time zero. Nevertheless the dynamics is not factorized with respect to the coordinates R and r. The mutual interaction of the two particles, described by the static δ-like potential in the relative coordinate, will eventually produce correlations between the positions of the two particles.
Expressed in the language of weighted Sobolev spaces $H^{m,s}$ (see e.g. [55])

$$H^{m,s}(\mathbb{R}^d) \equiv \left\{ u \in L^2(\mathbb{R}^d) : \left\| \left(1 + |\cdot|^2\right)^{\frac{s}{2}} (1-\Delta)^{\frac{m}{2}} u \right\|_{L^2(\mathbb{R}^d)} < +\infty \right\}$$

with $L^2_s(\mathbb{R}^d) = H^{0,s}(\mathbb{R}^d)$ and $H^m(\mathbb{R}^d) = H^{m,0}(\mathbb{R}^d)$, we will assume that initial state satisfies

Condition 1. $\varphi(R) \in H^{1,1}(\mathbb{R}^3)$ and $\chi(r) \in H^{1,1}(\mathbb{R}^3) \cap H^2(\mathbb{R}^3)$.

Our main result is expressed in the following theorem where we indicate with $\|\cdot\|$ the $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$-norm.

Theorem 2.1. *There exist two constants $A > 0$ and $B > 0$ such that for any initial state (2.13) satisfying condition 1 and any fixed $\alpha > 0$ and $t > 0$, one has*

$$\|\Psi(t) - \Psi^a(t)\| \leq A\left(\frac{\varepsilon}{t}\right)^{\frac{3}{4}} + B\varepsilon \tag{2.14}$$

where

$$\Psi^a(t) = e^{-it\mathbf{H}^a}\Psi_0^a \tag{2.15}$$

$$\mathbf{H}^a = H \otimes \mathbb{I} + \mathbb{I} \otimes H^\varepsilon \tag{2.16}$$

$$\Psi_0^a(R, r) = \varphi(R)\left[\left(\Omega_+^R\right)^{-1}\chi\right](r) \tag{2.17}$$

and the constants A *and* B *depend only on the initial state and on the constant* α.

The result of theorem 2.1 expressed by (2.15), (2.16), (2.17) can be thought as an exact formulation of the Joos and Zeh conjecture (2.1) for the special case of point interactions in three dimensions. As stressed by many authors (see e.g. [51], [27], [23], [3],) formula (2.1) can not be correct, as it stands, inasmuch as one is looking for a relation between initial and scattering states and not between *in* and *out* states. Roughly speaking (2.17) shows that the approximation formula holds true if in (2.1) the scattering matrix S^R is replaced with the wave operator $(\Omega_+^R)^{-1}$
The proof of theorem 2.1 is in appendix B.

2.2 Decoherence induced by scattering

We want to apply the results obtained in theorem 2.1 to the analysis of the decoherence effects induced by a single scattering event at the level of approximation of the dynamics given by the Joos and Zeh formula. As it was done in the one dimensional case [23], the estimate allows to compute how much quantum interference observed in the evolution of the state of the heavy particle, initially in a superposition state, is decreased by the presence of the light particle. We will interpret the decreasing of interference as a sign of a more classical behavior of the heavy particle.
The reduced density matrix for the heavy particle in the spatial coordinates representation is the positive, trace class operator $\rho_\alpha(t)$ in $L^2(\mathbb{R}^3)$ with $\mathrm{Tr}\,\rho_\alpha(t) = 1$ with integral kernel

$$\rho_\alpha(t; R, R') = \int_{\mathbb{R}^3} dr\, \Psi(t; R, r)\overline{\Psi}(t; R', r) \tag{2.18}$$

where $\Psi(t; R, r)$ is the solution of problem (2.12), (2.13).
In the small mass ratio limit, using the results contained in theorem 2.1, one easily obtains the following approximation for the density matrix (2.18)

$$\rho^a(t) = e^{-itH}\rho_0^a e^{itH} \tag{2.19}$$

where

$$\rho_0^a(R, R') = \varphi(R)\overline{\varphi}(R')\mathcal{I}(R, R') \tag{2.20}$$

$$\mathcal{I}(R, R') = ((\Omega_+^R)^{-1}\chi, (\Omega_+^{R'})^{-1}\chi) \tag{2.21}$$

It is easily seen that the following proposition holds

Proposition 2.1.1. Under the same assumptions of the theorem 2.1 one has

$$\text{Tr } |\rho_\alpha(t) - \rho^a(t)|^{\frac{1}{2}} \leq A \left(\frac{\varepsilon}{t}\right)^{\frac{3}{4}} + B\varepsilon \tag{2.22}$$

Without interaction the dynamics of the heavy particle is described by the reduced density matrix $\rho(t)$ obtained from the free evolution of the density matrix $\rho_0(R, R') = \varphi(R)\overline{\varphi}(R')$. Being $\rho_0(R, R')$ a projector operator one has

$$\text{Tr}(\rho(t))^2 = \text{Tr}(\rho_0)^2 = 1 \tag{2.23}$$

The amount of entanglement due to the interaction at the order of approximation of the Joos and Zeh formula is expressed by the term $\mathcal{I}(R, R')$ in the initial density matrix. Given the unitarity of the operators $(\Omega_+^R)^{-1}$ it is obvious that for $R \neq R'$ one has $|\mathcal{I}(R, R')| < 1$. This implies that

$$\text{Tr}(\rho^a(t))^2 = \text{Tr}(\rho_0^a)^2 < 1 \tag{2.24}$$

which in turns means that the reduced density matrix (2.19) describes a mixed state.
In addition to these immediate consequences of the unitarity of $(\Omega_+^R)^{-1}$ it is in principle possible in our specific model to compute explicitly $\mathcal{I}(R, R')$.
Given the unitarity of the Fourier transform and the definition of $(\Omega_+^R)^{-1}$ we can write

$$\mathcal{I}(R, R') = (\mathcal{F}_+^R \chi, \mathcal{F}_+^{R'} \chi) \tag{2.25}$$

We introduce the notation

$$\mathcal{F}_+^R = \mathcal{F} + K_R \tag{2.26}$$

where $\mathcal{F}$ is the usual Fourier transform and K_R is the operator

$$[K_R\chi](k) = \int_{\mathbb{R}^3} \frac{dr}{(2\pi)^{\frac{3}{2}}} \frac{e^{-ikR}}{4\pi\alpha - i|k|} \frac{e^{i|k||r-R|}}{|r-R|} \chi(r) \tag{2.27}$$

with this notation

$$\mathcal{I}(R, R') = (\chi, \chi) + (K_R\chi, \mathcal{F}\chi) + (\mathcal{F}\chi, K_{R'}\chi) + (K_R\chi, K_{R'}\chi) \tag{2.28}$$

Notice that because the unitarity of $(\Omega_+^R)^{-1}$, $\mathcal{I}(R, R) = (\chi, \chi)$ and the (2.28) implies

$$(K_R\chi, \mathcal{F}\chi) = -(\mathcal{F}\chi, K_R\chi) - (K_R\chi, K_R\chi) \tag{2.29}$$

To get an estimate for the amount of decoherence we consider a normalized state $(\chi, \chi) = 1$ and compute the quantity $1 - \mathcal{I}(R, R')$. From (2.28) and (2.29) we obtain

$$1 - \mathcal{I}(R, R') = (\mathcal{F}\chi, (K_R - K_{R'})\chi) + (K_R\chi, (K_R - K_{R'})\chi) \tag{2.30}$$

We will analyze (2.30) in the particular relevant case in which the initial state of the light particle is given by a symmetric wave packet centered at the origin, in particular let us choose

$$\chi(r) = \frac{e^{-\frac{|r|^2}{2\sigma^2}}}{(\pi\sigma^2)^{\frac{3}{4}}} \tag{2.31}$$

We will address our efforts on the special case in which $R' = -R$ and we will evaluate $\mathcal{I}(R,-R)$. It is easy to see that for every state such that $\chi(r) = \chi(-r)$

$$(\mathcal{F}\chi, (K_R - K_{-R})\chi) = 0 \tag{2.32}$$

Under the same assumption on $\chi(r)$ the second term in the r.h.s. of (2.30) can be written as

$$\begin{aligned}(K_R\chi, (K_R - K_{-R})\chi) = &\int_{\mathbb{R}^3} \frac{dk}{(2\pi)^3} \frac{1 - e^{2ikR}}{(4\pi\alpha)^2 + |k|^2} \times \\ &\times \int_{\mathbb{R}^3} dr \frac{e^{-i|k||r|}}{|r|} \overline{\chi}(r+R) \int_{\mathbb{R}^3} dr' \frac{e^{i|k||r'|}}{|r'|} \chi(r'+R)\end{aligned} \tag{2.33}$$

The two integrals in r and r' in the r.h.s. of the last expression are one the complex conjugate of the other. Using the specific form (2.31) of $\chi(r)$ we obtain

$$\begin{aligned}\left| \int dr \frac{e^{-i|k||r|}}{|r|} \overline{\chi}(r+R) \right|^2 = &\, 2\pi^{\frac{3}{2}} \frac{\sigma^3}{|R|^2} e^{-|k|^2\sigma^2} \times \\ &\times \left| e^{i|k||R|} erf(z) + e^{-i|k||R|} \overline{erf(z)} - 2i \sin |k||R| \right|^2\end{aligned} \tag{2.34}$$

where $z = \frac{|R| + i|k|\sigma^2}{\sqrt{2}\sigma}$. Inserting this in (2.33) and integrating on the angular part of k we have

$$\begin{aligned}1 - \mathcal{I}(R,-R) = &\frac{\sigma^3}{|R|^2\sqrt{\pi}} \int_0^\infty d|k| \frac{|k|^2}{(4\pi\alpha)^2 + |k|^2} \left(1 - \frac{\sin(2|k||R|)}{2|k||R|} \right) e^{-|k|^2\sigma^2} \times \\ &\times \left| e^{i|k||R|} erf(z) + e^{-i|k||R|} \overline{erf(z)} - 2i \sin |k||R| \right|^2\end{aligned} \tag{2.35}$$

Expression (2.35) clearly shows that for every R one has $1 - \mathcal{I}(R,-R) \geq 0$, moreover it is easy to see that, for fixed R, $1 - \mathcal{I}(R,-R)$ is a decreasing function of α. For this reason we focus our attention on the evaluation of (2.35) when $\alpha = 0$.

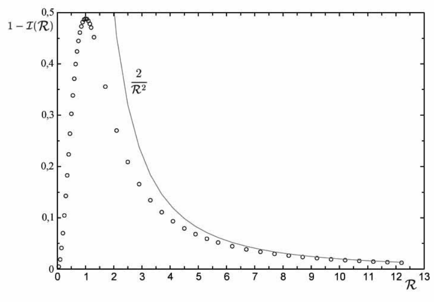
We define the dimensionless variables $\xi \equiv |k||R|$ and $\mathcal{R} \equiv |R|/\sigma$ and we pose $\mathcal{I}(R,-R) = \mathcal{I}(\mathcal{R})$. With this notation one has

$$\begin{aligned}1 - \mathcal{I}(\mathcal{R}) = &\frac{1}{|\mathcal{R}|^3\sqrt{\pi}} \int_0^\infty d\xi \left(1 - \frac{\sin(2\xi)}{2\xi} \right) e^{-\frac{\xi^2}{\mathcal{R}^2}} \times \\ &\times \left| e^{i\xi} erf\left(\frac{\mathcal{R}}{\sqrt{2}} + \frac{i}{\sqrt{2}} \frac{\xi}{\mathcal{R}} \right) + e^{-i\xi} erf\left(\frac{\mathcal{R}}{\sqrt{2}} - \frac{i}{\sqrt{2}} \frac{\xi}{\mathcal{R}} \right) - 2i \sin \xi \right|^2\end{aligned} \tag{2.36}$$

Analyzing the asymptotics of the positive integral in (2.36) it is easy to check that $1 - \mathcal{I}(\mathcal{R})$ tends to zero as $1/\mathcal{R}^2$ when $\mathcal{R}$ grows to infinity and as $\mathcal{R}$ when $\mathcal{R}$ tends to zero.

It is more interesting to investigate the range of values of $\mathcal{R}$ for which quantum interference is expected. The integral in (2.36) is not computable in closed form; its numerically computed behavior as a function of the parameter $\mathcal{R}$ is given in the figure.

Together with the initial state (2.31) for the light particle, let us consider an initial state of the heavy particle which is a coherent superposition of two wave



packets concentrated in regions symmetrically placed around the origin, at a distance $|R|$ each one with average momentum $\pm p_0$ heading toward the origin. At a time approximately given by the classical flight time $|R|/|p_0|$ one expects quantum interference to take place for distances of the order of the dispersion of the two wave packets.
Formula (2.20) for the approximate initial density matrix suggests that if σ is of the same order of the distance of the wave packets a maximum decoherence effect will take place.

Joos and Zeh, in their seminal paper on the subject [29], proceeded from the single scattering event toward the analysis of the decoherence effects induced on the heavy particle by the interaction with a gas of light particles.
In the case of a large number of non interacting light particles one expects to be able to prove a generalization of theorem (2.1) in the direction suggested by Joos and Zeh. In turn this would imply a decoherence effect which is exponentially increasing with the number of the particles of the environment.
Although conceivably true on a heuristic basis, the above mentioned result is not easy to prove, taking into account the complete Schrödinger dynamics. In fact the light particles are coupled through the heavy one, in the sense that the dynamics is not factorized in any coordinate system.

Chapter 3

Spin Dependent Point Interactions

All the quantum particles when revealed by detectors exhibit classical trajectories. This phenomenon was first investigated by N.F. Mott in his work on the tracks left by α-particles in a Wilson chamber, his words well summarize the problem: "It is a little difficult to picture how it is that an outgoing spherical wave can produce a straight track; we think intuitively that it should ionise atoms at random throughout space", from the article *The Wave Mechanics of α-Ray Tracks*, 1929 [33].

In his analysis Mott deduced that to explain the appearing of straight tracks one has to take into account the environment represented by the atoms in the gas inside the Wilson chamber. By using the stationary Schrödinger equation, he showed that two atoms in the gas cannot both be ionized unless they lie in a straight line with the radioactive nucleus. The use of the stationary theory is questionable but Mott's idea was undoubtedly ingenious and in the spirit of the decoherence program.

Our investigations are addressed to the realization of a model of Wilson chamber. We propose a system in which the environment consists of an array of spins. A quantum particle, interacting with the spins via a spin dependent point potential, plays the role of the quantum subsystem under observation.

The high degree of computability of the dynamics generated by point Hamiltonians should allow to show that, because of the interaction with the spins, the reduced density matrix relative to the particle initially in a pure state dynamically evolves towards a statistical mixture.

A realistic measurement apparatus should consist of a large number of spins. The effect of the interaction should be a "small" perturbation of the "free" evolution. The particle should proceed almost freely while the state of the spins will change substantially.

Following the same strategy as in the analysis of decoherence induced by scattering we start from the study of the dynamics in the two body problem.

As a preliminary step we concentrate our attention on the characterization of all the possible spin dependent point interactions between one particle and one spin that can be obtained from an assigned "free" dynamics. Details on such characterization in one and three dimensions are given in appendix C.

In this chapter we analyze the dynamics generated by a class of Hamiltonians among the ones obtained in appendix C. Our results indicate that entanglement occurs and that decoherence effects can be explicitly computed.
The generalization to a system of N spins, which do not interact between them, seems to be feasible although not trivial. The work on this system is in progress. Formally the structure of the Hilbert space of our system is identical to the one proposed in [10] in the analysis of the interaction between a particle with spin 1/2 and a quantum dot. It is easy to establish a close analogy between the Hamiltonian analyzed in [10] and the one (in dimension one) proposed in our model.

3.1 Free dynamics

We consider a system consisting of a quantum particle and one spin localized in the point y. From the mathematical point of view the spin is treated as a vector in $\mathbb{C}^2$. This approach is usual in solid state physics to study impurities in superconductors.
The natural Hilbert space for our system is

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^2 \,, \tag{3.1}$$

where d is the dimension of the space.
In the following we will indicate a vector in $\mathcal{H}$ with a capital Greek letter. In our analysis we will use the decomposition formula

$$\Psi = \sum_{\sigma=\pm} \psi_\sigma(x) \otimes \chi_\sigma \qquad \Psi \in \mathcal{H} \tag{3.2}$$

where $\psi_\sigma(x) \in L^2(\mathbb{R}^d)$ while $\chi_\pm$ are the normalized vectors in $\mathbb{C}^2$ satisfying $\sigma_x \chi_\pm = \pm\chi_\pm$ and σ_x is the Pauli matrix that on the standard basis of the spin operator $\vec{\sigma}$ is expressed by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{3.3}$$

The scalar product in $\mathcal{H}$ is naturally defined by

$$\langle \Psi_1, \Psi_2 \rangle = \sum_{\sigma=\pm} (\psi_{1\sigma}, \psi_{2\sigma}) \qquad \Psi_1,\, \Psi_2 \in \mathcal{H} \tag{3.4}$$

where $(\cdot\,,\cdot)$ indicates the standard scalar product in $L^2(\mathbb{R}^d)$.
The choice of the "free" Hamiltonian for the spin part is arbitrary, we consider the case in which the "free" dynamics of the spin is generated by a term in the Hamiltonian of the whole system proportional to σ_x. The operator

$$D(H) = H^2(\mathbb{R}^d) \otimes \mathbb{C}^2 \qquad H = -\Delta \otimes \mathbb{I} + \mathbb{I} \otimes \alpha\, \sigma_x \qquad \alpha \in \mathbb{R} \,. \tag{3.5}$$

is self-adjoint. The action of H on a generic vector $\Psi \in \mathcal{H}$ can be written as

$$H\Psi = \sum_{\sigma=\pm} [(-\Delta + \sigma\alpha)\psi_\sigma](x) \otimes \chi_\sigma \tag{3.6}$$

The resolvent of H is

$$(H-z)^{-1}\Psi = \sum_{\sigma=\pm}[(-\Delta+\sigma\alpha-z)^{-1}\psi_\sigma](x)\otimes\chi_\sigma \qquad z\in\rho(H) \tag{3.7}$$

where $\rho(H)$ is the resolvent set of H and

$$[(-\Delta-\lambda)^{-1}\psi_\sigma](x) = \int_{\mathbb{R}^d} G^\lambda(x-x')\psi_\sigma(x')dx' \qquad \lambda\in\mathbb{C}\backslash\mathbb{R}^+ \tag{3.8}$$

with $G^\lambda(x)$ integral kernel of $(-\Delta-\lambda)^{-1}$

$$G^\lambda(x) = \begin{cases} i\dfrac{e^{i\sqrt{\lambda}|x|}}{2\sqrt{z}} & d=1 \\ \\ \dfrac{e^{i\sqrt{\lambda}|x|}}{4\pi|x|} & d=3 \end{cases} \qquad \lambda\in\mathbb{C}\backslash\mathbb{R}^+\ , \quad \mathrm{Im}\,(\sqrt{\lambda})>0 \tag{3.9}$$

The spectrum o f H is easily obtained from (3.7) and from the spectral structure of the "free" Schrödinger operator. The point spectrum of H is empty, $\sigma_{pp}(H) = \varnothing$ and the essential spectrum is only absolutely continuous

$$\sigma(H) = \sigma_{ess}(H) = \sigma_{ac}(H) = [-|\alpha|, +\infty)\,. \tag{3.10}$$

Notice that the part of the (continuous) spectrum $[|\alpha|,+\infty)$ is four fold degenerate. While the part of the (continuous) spectrum $[-|\alpha|,|\alpha|)$ is only two fold degenerate.
By using the property of the Laplace transform $\mathcal{L}^{-1}\Big(\mathcal{L}(f)(\cdot+\alpha)\Big)(\tau) = e^{-\alpha\tau}f(\tau)$ and from the expression of the resolvent of H one obtains the explicit form for the propagator e^{-iHt}. The solution of the Cauchy problem

$$\begin{cases} i\dfrac{d\Psi^t}{dt} = H\Psi^t \\ \Psi^{t=0} = \Psi^0 \end{cases} \tag{3.11}$$

is given by

$$\Psi^t = e^{-iHt}\Psi^0 = \sum_{\sigma=\pm}\left(U^t\psi^0_\sigma\right)(x)\otimes e^{-i\sigma\alpha t}\chi_\sigma\,, \tag{3.12}$$

where

$$\left(U^t f\right)(x) = \int_{\mathbb{R}^d}\frac{e^{i\frac{|x-x'|^2}{4t}}}{(4\pi i t)^{\frac{d}{2}}}f(x')dx' \tag{3.13}$$

The spin can be in a superposition of states χ_+ and χ_-.

3.2 Interacting dynamics

We call point perturbation of Hamiltonian (3.5) every self-adjoint operator which coincides with H on vectors in $\mathcal{H}$ for which the wave function part has no support in the point y.

In appendix C we discuss in detail the characterization of the family of self-adjoint perturbations of the operator H obtained with the theory of self-adjoint extensions. In dimension one elements in such family are identified by sixteen real parameters while in dimension three only four real parameters are required. In this section we state the main results about the spectral structure and the propagator of the subfamily of self-adjoint perturbations of H corresponding to a generalization of the δ-like interactions discussed in chapter 1. In our model the "intensity" of the point potential depends on the value of the x-component of the spin. As we will see in the following section this occurrence generate entanglement between the particle and spin.
We indicate with $\hat{H}$ the operators in this subfamily. The following theorem is obtained by direct construction in appendix C.

Theorem 3.1. *The operator* $\hat{H}$

$$D(\hat{H}) = \Big\{\Psi \in \mathcal{H} : \ \Psi = \Psi^z + \sum_{\sigma=\pm} (\Gamma_\sigma(z))^{-1} \psi^z_\sigma(y) \Phi^z_\sigma ; \ \Psi^z \in D(H) \\ \Psi^z = \sum_\sigma \psi^z_\sigma(x) \otimes \chi_\sigma \, ; \ -\infty < \gamma_\pm \leq \infty \, , \ z \in \rho(\hat{H}) \Big\} \tag{3.14}$$

$$(\hat{H} - z)\Psi = (H - z)\Psi^z \qquad z \in \rho(\hat{H}) \tag{3.15}$$

with

$$(\Gamma_\pm(z))^{-1} = \begin{cases} -\dfrac{2\gamma_\pm \sqrt{z \mp \alpha}}{i\gamma_\pm + 2\sqrt{z \mp \alpha}} & d = 1 \\ \dfrac{4\pi}{4\pi\gamma_\pm - i\sqrt{z \mp \alpha}} & d = 3 \end{cases} \qquad z \in \rho(\hat{H}) \, , \quad Im(\sqrt{z \mp \alpha}) > 0 \tag{3.16}$$

and

$$\Phi^z_\pm = G^{z \mp \alpha}(x - y) \otimes \chi_\pm \qquad z \in \rho(\hat{H}) \tag{3.17}$$

where $G^z(x)$ *is the integral kernel of the Laplacian which expression in dimensions one and three is given in (3.9), is self-adjoint and its resolvent is*

$$(\hat{H} - z)^{-1} = (H - z)^{-1} + \sum_{\sigma=\pm} (\Gamma_\sigma(z))^{-1} \langle \Phi^{\bar{z}}_\sigma, \cdot \rangle \Phi^z_\sigma \qquad z \in \rho(\hat{H}). \tag{3.18}$$

It is a simple exercise, and it is done in appendix C to verify that in dimension one vectors in $D(\hat{H})$ satisfy

$$\psi'_\pm(y^+) - \psi'_\pm(y^-) = \gamma_\pm \psi_\pm(y) \tag{3.19}$$

where $\psi_\pm(x)$ individuates the wave function part relative to $\chi_\pm$ of the generic vector $\Psi \in D(\hat{H})$. While in dimension three the wave function part of a vector in $D(\hat{H})$ has a singularity of order $|x - y|^{-1}$ and

$$\psi_\pm(x) = \psi^z_\pm(x) + \frac{q_\pm}{4\pi|x - y|} e^{i\sqrt{z \mp \alpha}|x - y|} \qquad \psi^z_\pm(x) \in H^2(\mathbb{R}^3) \\ z \in \rho(\hat{H}) \, , \quad \mathrm{Im}\,(\sqrt{z \mp \alpha}) > 0 \tag{3.20}$$

with

$$q_\pm = \frac{4\pi\psi^z_\pm(y)}{4\pi\gamma_\pm - i\sqrt{z \mp \alpha}} \tag{3.21}$$

notice that $q_\pm$ do not depend on z.
The structure of $\hat{H}$ in one and three dimensions is very similar to the well known operators H^{1d}_α and H^{3d}_α introduced in chapter 1, this makes very easy to know the spectral structure of $\hat{H}$ and to find an explicit expression for the propagator $e^{-i\hat{H}t}$.

Theorem 3.2. *Both in one and three dimensions the essential spectrum is only absolutely continuous and*

$$\sigma_{ess}(\hat{H}) = \sigma_{ac}(\hat{H}) = [-|\alpha|, +\infty)\,. \tag{3.22}$$

If $\gamma_+ < 0$ and/or $\gamma_- < 0$ then

$$E_+ = \begin{cases} \alpha - \dfrac{\gamma_+^2}{4} \\ \alpha - (4\pi\gamma_+)^2 \end{cases} \quad \text{and/or} \quad E_- = \begin{cases} -\alpha - \dfrac{\gamma_-^2}{4} & d = 1 \\ -\alpha - (4\pi\gamma_-)^2 & d = 3 \end{cases} \tag{3.23}$$

are eigenvalues.
If $d = 1$ for $\alpha > 0$ and $-2\sqrt{2\alpha} < \gamma_+ < 0$ the eigenvalue E_+ is embedded in the continuous spectrum, for $\alpha < 0$ and $-2\sqrt{2|\alpha|} < \gamma_- < 0$ the eigenvalue E_- is embedded in the continuous spectrum.
If $d = 3$ for $\alpha > 0$ and $-\sqrt{2\alpha} < 4\pi\gamma_+ < 0$ the eigenvalue E_+ is embedded in the continuous spectrum, for $\alpha < 0$ and $-\sqrt{2|\alpha|} < 4\pi\gamma_- < 0$ the eigenvalue E_- is embedded in the continuous spectrum.
The normalized eigenvectors relative to the eigenvalues E_+ and E_- are for $d = 1$

$$\Phi_{E_+} = \sqrt{\frac{|\gamma_+|}{2}} e^{-\frac{|\gamma_+|}{2}|x-y|} \otimes \chi_+ \; ; \qquad \Phi_{E_-} = \sqrt{\frac{|\gamma_-|}{2}} e^{-\frac{|\gamma_-|}{2}|x-y|} \otimes \chi_- \tag{3.24}$$

while for $d = 3$

$$\Phi_{E_+} = \sqrt{2|\gamma_+|}\frac{e^{-4\pi|\gamma_+|\,|x-y|}}{|x-y|} \otimes \chi_+ \; ; \quad \Phi_{E_-} = \sqrt{2|\gamma_-|}\frac{e^{-4\pi|\gamma_-|\,|x-y|}}{|x-y|} \otimes \chi_- \tag{3.25}$$

The proof of theorem 3.2 is a simple generalization of the analogous proofs about the spectrum of the singular perturbations of the Laplacian in one and three dimensions that one can find in [9].
The solution of the Cauchy problem

$$\begin{cases} i\dfrac{d\hat{\Psi}^t}{dt} = \hat{H}\hat{\Psi}^t \\ \hat{\Psi}^{t=0} = \Psi^0 \end{cases} \tag{3.26}$$

is given by

$$\hat{\Psi}^t = e^{-i\hat{H}t}\Psi^0 = \sum_{\sigma=\pm} \left(U^t_{\gamma_\sigma}\psi^0_\sigma\right)(x) \otimes e^{-i\sigma\alpha t}\chi_\sigma \tag{3.27}$$

where for $d = 1$

$$U^t_{\gamma_\pm}(x,x') = U^t(x-x') + \\ + \begin{cases} -\dfrac{\gamma_\pm}{2}\displaystyle\int_0^\infty e^{-\frac{\gamma_\pm}{2}u} U^t(u+|x-y|+|x'-y|)du & \gamma_\pm > 0 \\ 0 & \gamma_\pm = 0 \\ \dfrac{|\gamma_\pm|}{2} e^{i\frac{|\gamma_\pm|^2}{4}t} e^{-\frac{|\gamma_\pm|}{2}|x-y|} e^{-\frac{|\gamma_\pm|}{2}|x'-y|} + & \\ \quad + \dfrac{\gamma_\pm}{2}\displaystyle\int_0^\infty e^{\frac{\gamma_\pm}{2}u} U^t(u-|x-y|-|x'-y|)du & \gamma_\pm < 0 \end{cases} \tag{3.28}$$

while for $d = 3$

$$U^t_{\gamma_\pm}(x,x') = U^t(x-x') + \frac{2it}{|x-y||x'-y|} U^t(|x-y|+|x'-y|) + \\ + \begin{cases} -\dfrac{8\pi\gamma_\pm it}{|x-y||x'-y|}\displaystyle\int_0^\infty e^{-4\pi\gamma_\pm u} U^t(u+|x-y|+|x'-y|)du & \gamma_\pm > 0 \\ 0 & \gamma_\pm = 0 \\ 2|\gamma_\pm| e^{4\pi i|\gamma_\pm|^2 t} \dfrac{e^{-4\pi|\gamma_\pm|\,|x-y|}}{|x-y|} \dfrac{e^{-4\pi|\gamma_\pm|\,|x'-y|}}{|x'-y|} + & \\ \quad + \dfrac{8\pi\gamma_\pm it}{|x-y||x'-y|}\displaystyle\int_0^\infty e^{4\pi\gamma_\pm u} U^t(u-|x-y|-|x'-y|)du & \gamma_\pm < 0 \end{cases} \tag{3.29}$$

where $U^t(x)$ is defined in (3.13). The derivations of propagators $U^t_{\gamma_\pm}(x,x')$ is in [43], [6] and [7].

3.3 Application to decoherence

We are interested in showing that because of interaction some entanglement occurs also when the initial state is factorized. In the spirit of the decoherence program we analyze the time evolution of entanglement and the effects of decoherence obtained by tracing out the environment.
Consider the initial state

$$\Psi^0 = \psi^0(x) \otimes \left[\frac{\chi_+ + \chi_-}{\sqrt{2}}\right] \tag{3.30}$$

where $\psi^0(x) \in L^2(x)$ and $\|\psi^0\| = 1$.
The "free" evolution of Ψ_0 given by the Hamiltonian H is easily obtained by applying formula (3.12)

$$\Psi^t = \left(U^t\psi^0\right)(x) \otimes \left[\frac{e^{-i\alpha t}\chi_+ + e^{i\alpha t}\chi_-}{\sqrt{2}}\right] \tag{3.31}$$

We will use the formalism of the density matrices. In the "free" case the density matrix associated with Ψ^t is

$$\rho(t) = \Psi^t \langle \Psi^t, \cdot\, \rangle \tag{3.32}$$

In the standard representation of the algebra of Pauli matrices in which $\chi_+ = (1/\sqrt{2}, 1/\sqrt{2})$ and $\chi_- = (1/\sqrt{2}, -1/\sqrt{2})$, the reduced density matrix obtained from $\rho(t)$ by tracing out the wave function part is

$$\rho_{red,\chi}(t) = \mathrm{Tr}_{L^2}(\rho(t)) = \frac{1}{2}\begin{pmatrix} 1 & e^{-2i\alpha t} \\ e^{2i\alpha t} & 1 \end{pmatrix} \tag{3.33}$$

Since there is no interaction between the spin and the particle $\rho_{red,\chi}$ is still a projector and still represents a pure state. In particular $\mathrm{Tr}_{\mathbb{C}^2}(\rho^2_{red,\chi}(t)) = 1$. As expected no effect of decoherence is produced if there is no interaction.
The same result is obtained by tracing out the subsystem consisting of the spin, in fact

$$\rho_{red,\psi}(t; x, x') = \mathrm{Tr}_{\mathbb{C}^2}(\rho(t)) = \left(U^t\psi^0\right)(x)\overline{(U^t\psi^0)}(x') \tag{3.34}$$

and $\mathrm{Tr}_{L^2}(\rho^2_{red,\psi}(t)) = 1$.
If the generator of the dynamics is $\hat{H}$ things are quite different. Suppose that $\gamma_+ \neq \gamma_-$, then from formula (3.27) it is clear that interaction generate entanglement between the particle and the spin in fact the state

$$\hat{\Psi}^t = \left(U^t_{\gamma_+}\psi^0\right)(x) \otimes \frac{e^{-i\alpha t}\chi_+}{\sqrt{2}} + \left(U^t_{\gamma_-}\psi^0\right)(x) \otimes \frac{e^{i\alpha t}\chi_-}{\sqrt{2}} \tag{3.35}$$

is no more factorized. We expect that by tracing out the spins (or the particle) we will obtain a reduced density matrix that does not describe a pure state but a statistical mixture. This is true, in fact, proceeding as in (3.32) and (3.33) one has

$$\hat{\rho}(t) = \hat{\Psi}^t \langle \hat{\Psi}^t, \cdot \,\rangle \tag{3.36}$$

and

$$\hat{\rho}_{red,\chi}(t) = \mathrm{Tr}_{L^2}(\hat{\rho}(t)) = \frac{1}{2}\begin{pmatrix} 1 & u(t)\, e^{-2i\alpha t} \\ \overline{u(t)}\, e^{2i\alpha t} & 1 \end{pmatrix} \tag{3.37}$$

with

$$u(t) = \int dx \left(U^t_{\gamma_+}\psi_0\right)(x)\overline{\left(U^t_{\gamma_-}\psi_0\right)}(x) \tag{3.38}$$

If $\gamma_+ \neq \gamma_-$ because the unitarity in $L^2(\mathbb{R}^d)$ of $U^t_{\gamma_+}$ and $U^t_{\gamma_-}$ one has

$$\mathrm{Tr}_{\mathbb{C}^2}(\rho^2_{red}(t)) = \frac{1}{2} + \frac{|u(t)|^2}{2} < 1 \tag{3.39}$$

In principle, given ψ_0, function $u(t)$ is computable at any time.
Notice that the same result holds if we consider the reduced density matrix obtained by tracing out the spin part,

$$\begin{aligned}\hat{\rho}_{red,\psi}(t; x, x') = \mathrm{Tr}_{\mathbb{C}^2}(\hat{\rho}(t)) =& \frac{1}{2}\left(U^t_{\gamma_+}\psi^0\right)(x)\overline{\left(U^t_{\gamma_+}\psi^0\right)}(x') + \\ &+ \frac{1}{2}\left(U^t_{\gamma_-}\psi^0\right)(x)\overline{\left(U^t_{\gamma_-}\psi^0\right)}(x')\end{aligned} \tag{3.40}$$

and

$$\mathrm{Tr}_{L^2}(\rho^2_{red,\psi}(t)) = \mathrm{Tr}_{\mathbb{C}^2}(\rho^2_{red}(t)) = \frac{1}{2} + \frac{|u(t)|^2}{2} < 1 \tag{3.41}$$

Notice that interaction it is not the only requirement to have entanglement. If $\gamma_+ = \gamma_-$ no decoherence can be observed because the particle is unable to distinguish the state of the spin.
Moreover if the initial state is

$$\Psi^0 = \psi^0(x) \otimes \chi_+ \tag{3.42}$$

the state persists to be factorized and no entanglement is produced. Decoherence does not take place because there is no transfer of information between the subsystems.
The results obtained suggest to increase efforts in the analysis of the systems proposed. Analytic estimates of $u(t)$ are of interest both in one and three dimensions. The next step should be the generalization to a system of N spins. The analysis of self-adjoint perturbations of H different from $\hat{H}$ is of some interest. In our opinion more attention should be payed to Hamiltonians that do not commute with σ_x.

Part II

Point Interactions in Acoustics

Singular extensions of symmetric operators turned out to be a powerful tool in modelling classical systems made up of a compressible fluid and several mechanical oscillators, coupled to the acoustic field they produce in the fluid.
The physical system under study was suggested by the appearance in 1999 of a paper by J. D. Templin [52]. In that paper the author analyzed the dynamics of a simple model of a spherical oscillator interacting with the acoustic field it generates. The pressure field at the surface of the sphere completely characterizes the contact forces responsible of the interaction between source and field. The existence of a spherically symmetric radiation field, the *acoustic monopole*, makes possible detailed analysis of the field emitted by the acoustic monopole. Explicitly computing both its radiation and near-field components Templin noticed that a deduction of the *reaction field* obtained from the emitted radiation power, therefore neglecting the near field component, brings to an equation for the radius of the oscillating sphere showing *runaway solutions*, i.e. solutions for which the acceleration increases beyond any bound even in the absence of external fields.
Runaway solutions are well known in classical electromagnetism where all attempts to construct a complete, covariant, causal, divergence free theory for the evolution of the fields together with their sources were unsuccessful up to now. Actually it is hard to say that there is a single case in classical or in quantum physics in which this problem was completely solved.
Whereas theories with extended rigid charges are quite well understood both at the classical and the quantum level (see e.g. the recent book [50] for a systematic introduction to the subject and for a long list of references), there is no mathematically consistent theory of point charges interacting with their own electromagnetic field. Indeed Newton equations with Lorentz force require the fields to be evaluated at the particle positions, and this produces infinities due to the presence of the point-like sources. These difficulties directly lead to the need of mass renormalization. In his seminal paper Dirac [22] (also see [28], [30], [32]), without using Lorentz force but exploiting the conservation of energy and momentum and considering their flow through a thin tube of radius r, derived an equation for the motion of a charged point particle (the Lorentz-Dirac equation). As Dirac himself pointed out the equation obtained in the limit $r \downarrow 0$, together with the mass renormalization, leads to the presence of runaway solutions.
An approach based on the theory of singular perturbations of the free dynamics was initiated in [35] and [36] for the case of classical electrodynamics of a point particle in the dipole (or linearized) case. Here the generator of the limit dynamics of both the field and the particle appears to be a singular perturbation of the generator of the free dynamics. The phenomenological mass plays the role of the parameter describing a suitable family of self-adjoint extensions and the boundary condition naturally appearing in the domain of the generator results to be nothing else that a regularized (and linearized) version of the usual velocity-momentum relation in the presence of an electromagnetic field. In this framework runaway solutions are unavoidable because a negative eigenvalue appears in the spectrum of the generator after mass renormalization.
In analogy with what was done for the electromagnetic case in [35] we provide a formalization of the problem of oscillators coupled with their acoustic field in terms of singular perturbations of the generator of the free dynamics. As an immediate consequence of the third Newton's law and of the assumption of

persistent contact between the fluid and the surface of the oscillators, the total energy, sum of the (positive) energy of the acoustic field E_{ac} and the (positive) energy of the oscillators E_{osc}, is a constant of motion. As an immediate consequence one can exclude the existence of runaway solutions in this case. Moreover, lacking a mechanism of reflection of the acoustic waves at some exterior boundary, the motion of the oscillators should be damped and the energy should finally diffuse over the field degrees of freedom, for almost every initial condition. The situation is reminiscent of the one investigated in [47], [48] and [49] about the diffusion of energy from bound states to continuous states triggered by time dependent perturbations in quantum and classical systems even though in our system there is no external potential the interaction being given by internal forces.

In chapter 4 we state our results in one dimension. In this case it is possible to study a system made up of several mechanical oscillators coupled to the acoustic field in the fluid surrounding them for different settings of the oscillators array. The generalization to three dimensions is not straightforward. From one side a model of a physically relevant, symmetric, mechanical oscillator with finite degrees of freedom is lacking. On the other side point perturbations of the free dynamics are much more singular in higher dimensions.

Chapter 4

Point Interactions in Acoustics: One Dimensional Models

We analyze the dynamics of a one dimensional system made up of mechanical oscillators interacting with the acoustic field they produce in the fluid surrounding them.
We suggest a formalization of the problem in terms of singular perturbations of a free skew-adjoint operator. In our setting the dynamics of the whole system (mechanical oscillators and acoustic field) is generated by a strongly continuous unitary group of evolution.
Although in dimension one the model is more simple of the three dimensional one introduced by Templin in 1999 [52] the formalization proposed is completely new. With our approach the description of a system with finite oscillators becomes trivial and the generalization of the results about the damping of the oscillations, obtained by direct evaluation in the simple case of a single oscillator, is an immediate consequence of the unitarity of the evolution group generating the dynamics.
The generalization of the construction to the case of infinitely many sources is given. In the case of sources periodically placed on the real line it is possible to obtain detailed results on the characteristic band structure of the spectrum of the generator of the dynamics.
The results obtained are used to analyze a one-dimensional problem of homogenization.

4.1 The acoustic monopole in one dimension

We give a detailed description of our model in the simplest case of one oscillator coupled with the acoustic field.
Consider an infinite pipe filled with a non viscous, compressible fluid. We suppose that there is no friction between the fluid and the pipe and we choose a coordinate system with the x-axis parallel to the axis of the pipe. The mechanical oscillator is made up of a very thin wall of mass M positioned in the pipe

perpendicularly to the axis in $x = 0$. The thin wall is connected to a spring of elastic constant K. We analyze only one dimensional cases, hence the acoustic field is described by the pressure field $p(x,t)$ and the velocity field $v(x,t)$. The motion of the mechanical oscillator is described through the position and the velocity of the thin wall.
The field $p(x,t)$ represents deviations of the pressure in the point x at time t with respect to an equilibrium pressure P_0. In the linearized acoustics regime the continuity equation, the Newton's second law and the adiabatic equation of state read

$$\frac{\partial \rho}{\partial t} + \rho_0 \frac{\partial v}{\partial x} = 0 \,, \quad \rho_0 \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x} \,, \quad p = a^2 \rho \,, \tag{4.1}$$

where $\rho(x,t)$ is the deviation of the density in the point x at time t with respect to the equilibrium density ρ_0 and a is the velocity of sound in the fluid.
Then we have for $p(x,t)$ and $v(x,t)$ the following coupled differential equations

$$\frac{\partial p}{\partial t} = -a^2 \rho_0 \frac{\partial v}{\partial x} \,, \quad \frac{\partial v}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x} \,. \tag{4.2}$$

We consider only small oscillations of the thin wall around its equilibrium position $x = 0$, we indicate with $y(t)$ the displacement of the wall from its equilibrium position at time t and we suppose that the wall remains always in contact with the fluid

$$v(y(t),t) = \frac{dy(t)}{dt} \qquad \forall t \geq 0 \,. \tag{4.3}$$

Notice that we consider a wall of zero thickness. We make the approximation $v(y(t),t) \simeq v(0,t)$ and condition (4.3) becomes

$$v(0,t) = \frac{dy(t)}{dt} \qquad \forall t \geq 0 \,. \tag{4.4}$$

The equation of motion for the position of the thin wall $y(t)$ is

$$M\ddot{y}(t) = -Ky(t) - S\left(p(0^+,t) - p(0^-,t)\right) \tag{4.5}$$

where S is the area of the transversal section of the pipe and we made the approximation $p(y^{\pm}(t),t) \simeq p(0^{\pm},t)$.
The total energy of the system is given by

$$E_{tot} = E_{ac} + E_{osc} \tag{4.6}$$

with

$$E_{ac} = \frac{S}{2a^2\rho_0} \int_{-\infty}^{\infty} p(x)^2 dx + \frac{S\rho_0}{2} \int_{-\infty}^{\infty} v(x)^2 dx \tag{4.7}$$

$$E_{osc} = \frac{K}{2} y^2 + \frac{M}{2} \dot{y}^2 \,, \tag{4.8}$$

E_{ac} is the energy stored in the acoustic field while E_{osc} is the energy of the mechanical oscillator.
As the system is isolated the energy is constant. The motion of the wall produces acoustic waves thus transferring continuously energy from the oscillator to the acoustic field. One then expects that $y(t)$ decreases to zero when $t \to \infty$.

To evaluate the decay rate one have to solve the following Cauchy problem of coupled partial and ordinary differential equations with time dependent boundary conditions

$$\begin{cases} \dfrac{\partial p}{\partial t} = -a^2 \rho_0 \dfrac{\partial v}{\partial x} & \forall t \geq 0 \; \forall x \in \mathbb{R} \backslash \{0\} \\ \dfrac{\partial v}{\partial t} = -\dfrac{1}{\rho_0} \dfrac{\partial p}{\partial x} & \forall t \geq 0 \; \forall x \in \mathbb{R} \backslash \{0\} \\ \ddot{y}(t) = -\omega_0^2 y(t) - \dfrac{S}{M} \big(p(0^+, t) - p(0^-, t) \big) & \forall t \geq 0 \\ p(x, 0) = f(x) & \forall x \in \mathbb{R} \backslash \{0\} \\ v(x, 0) = g(x) & \forall x \in \mathbb{R} \backslash \{0\} \\ y(0) = y_0 & \\ \dot{y}(0) = \dot{y}_0 & \\ v(0, t) = \dot{y}(t) & \forall t \geq 0 \end{cases} \tag{4.9}$$

where $f(x)$ and $g(x)$ are two real functions and $\omega_0^2 = K/M$.
It is not hard to find the exact solution to problem (4.9) and to verify that if

$$f(x) \in C_0^2(\mathbb{R}) \, ; \; g(x) \in C_0^2(\mathbb{R}) \quad \text{and} \quad y_0 = \frac{1}{\omega_0^2 \rho_0} f'(0) \, ; \; \dot{y}_0 = g(0) \, , \tag{4.10}$$

than $y(t)$ and $\dot{y}(t)$ are both continuous and decrease exponentially to zero with decay constant $\tau = a \rho_0 S / M$. In spite of being a simple exercise, the exact computation of the solution of problem (4.2), (4.4), (4.5) and, in turn, of the damping rate of the oscillations rarely appears in textbooks, the details of the solution of Cauchy problem (4.9) are in [16].

4.2 Singular perturbations of the free dynamics

In this section we present a generalization of problem (4.9) formulated in terms of a unitary flow on a space of finite energy.
In analogy with what was done for the electromagnetic case in [35] we define the generator $\hat{A}$ of the interacting dynamics, as a singular perturbation of the generator of the free dynamics.
We consider a system of n thin walls positioned in the pipe perpendicularly to its axis. Let $\mathcal{S} = \{s_1, \ldots, s_n\} \subset \mathbb{R}$ be the set of equilibrium positions of the thin walls. The i-th thin wall, placed in s_i, has mass M_i and is connected to a spring of elastic constant K_i.
We will use a capital Greek letter to indicate a generic vector $(p, v, \underline{y}, \underline{z}) \in L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n$, where $L^2(\mathbb{R})$ is the space of square-integrable functions on the real line,

$$\underline{y} = y_1 \underline{e}_1 + \cdots + y_n \underline{e}_n \, , \quad \underline{z} = z_1 \underline{e}_1 + \cdots + z_n \underline{e}_n \tag{4.11}$$

and $\underline{e}_1, \ldots, \underline{e}_n$ is the canonical orthonormal base in $\mathbb{C}^n$.
Consider the Hilbert space

$$\mathcal{H} := L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \tag{4.12}$$

with the scalar product

$$\langle\langle \Psi_1, \Psi_2 \rangle\rangle \;=\frac{1}{a^2\rho_0}(p_1, p_) + \rho_0(v_1, v_2) + \frac{1}{S}\sum_{j=1}^{n} K_j\, \bar{y}_{1j} y_{2j} + M_j\, \bar{z}_{1j} z_{2j}\,, \quad (4.13)$$

where a, ρ_0, K_j, M_j, $1 \le j \le n$, are positive real constants representing the physical parameters previously defined, S is the area of the transversal section of the pipe, $(\cdot\,,\cdot)$ indicates the standard scalar product in $L^2(\mathbb{R})$ and $^-$ denotes complex conjugation.
The square norm of a vector Ψ, $\|\Psi\|^2 = \langle\langle \Psi, \Psi \rangle\rangle$, defines the total energy of the system in the state Ψ

$$E_{tot} = \frac{S}{2}\|\Psi\|^2 = E_{ac} + E_{osc} \quad (4.14)$$

where E_{ac} is the energy stored in the acoustic field while E_{osc} is the energy of the oscillators

$$E_{ac} = \frac{S}{2a^2\rho_0}\,(p,p) + \frac{\rho_0 S}{2}(v,v)\;; \quad E_{osc} = \frac{1}{2}\sum_{j=1}^{n}\left(K_j|y_j|^2 + M_j\,|z_j|^2\right)\,. \quad (4.15)$$

Define

$$\mathbf{L}\,(p, v, \underline{y}, \underline{z}) := \left(-a^2\rho_0\,\frac{dv}{dx},\; -\frac{1}{\rho_0}\,\frac{dp}{dx},\; \underline{z},\; -\sum_{j=1}^{n}\frac{K_j}{M_j}\,y_j\underline{e}_j\right) \qquad (p, v, \underline{y}, \underline{z}) \in \mathcal{H}\,. \quad (4.16)$$

Indicating with $\bar{H}^1(\mathbb{R})$ the homogeneous Sobolev space of locally square-integrable functions with square-integrable (distributional) derivative and with $H^1(\mathbb{R})$ the usual Sobolev space $H^1(\mathbb{R}) := \bar{H}^1(\mathbb{R}) \cap L^2(\mathbb{R})$, the operator A

$$D(A) := H^1(\mathbb{R}) \oplus H^1(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n \to \mathcal{H} \qquad A\Psi := \mathbf{L}\Psi \qquad \Psi \in D(A) \quad (4.17)$$

A is skew-symmetric and real, i.e. it preserves the (physical) linear subspace of real elements

$$\left\{(p, v, \underline{y}, \underline{z}) \in \mathcal{H} \,:\, p(x) \in \mathbb{R},\; v(x) \in \mathbb{R},\; \underline{y} \in \mathbb{R}^n,\; \underline{z} \in \mathbb{R}^n\right\}\,. \quad (4.18)$$

The resolvent of A is

$$(-A+\zeta)^{-1}(p, v, \underline{y}, \underline{z}) = \left(\rho_0\left(-\frac{d^2}{dx^2} + \frac{\zeta^2}{a^2}\right)^{-1}\left(-\frac{dv}{dx} + \frac{\zeta}{a^2\rho_0}\,p\right),\right.$$
$$\frac{1}{a^2\rho_0}\,\left(-\frac{d^2}{dx^2} + \frac{\zeta^2}{a^2}\right)^{-1}\left(-\frac{dp}{dx} + \zeta\rho_0 v\right),\; \sum_{j=1}^{n}\frac{M_j z_j + \zeta M_j y_j}{K_j + \zeta^2 M_j}\,\underline{e}_j\,, \quad (4.19)$$
$$\left.\sum_{j=1}^{n}\frac{-K_j y_j + \zeta M_j z_j}{K_j + \zeta^2 M_j}\,\underline{e}_j\right) \qquad (p, v, \underline{y}, \underline{z}) \in \mathcal{H},\; \zeta \in \mathbb{C}\backslash i\mathbb{R}\,.$$

Since $\mathrm{Ran}(-A \pm 1) = \mathcal{H}$, A is skew-adjoint.

Moreover the essential spectrum of A is purely absolutely continuous and

$$\sigma_{ess}(A) = \sigma_{ac}(A) = i\mathbb{R}\,, \quad \sigma_{pp}(A) = \left\{ \pm i \sqrt{\frac{K_j}{M_j}}\,,\ 1 \leq j \leq n \right\}. \tag{4.20}$$

Consider the linear, closed, densely defined, skew-symmetric operator A_0

$$D(A_0) = \Big\{ (p, v, \underline{y}, \underline{z}) \in H^1(\mathbb{R}) \oplus H^1(\mathbb{R}) \oplus \mathbb{C}^n \oplus \mathbb{C}^n : \\ v(s_j) = z_j,\ j = 1, \ldots, n \Big\} \tag{4.21}$$

$$A_0 \Psi = \mathbf{L}\Psi \quad \Psi \in D(A_0)$$

A is a skew-adjoint extension of A_0. We want to find all the skew-adjoint extensions of A_0 different from A which coincide with A on $D(A_0)$.
Since A_0 is a skew-symmetric operator formulas given in appendix A are slightly different. Equation (A.9) is substituted by

$$A_0^* \Phi^\zeta = \zeta \Phi^\zeta \qquad \Phi^\zeta \in D(A_0^*),\ \zeta \in \mathbb{C}\backslash i\mathbb{R} \tag{4.22}$$

It is easy to verify that for ζ fixed there are n independent solutions of equation (4.22), they read

$$G_\zeta^j(x) = \left(-\mathcal{G}'_\zeta(x - s_j)\,, \frac{\zeta}{a^2 \rho_0}\, \mathcal{G}_\zeta(x - s_j)\,, \frac{-S}{K_j + \zeta^2 M_j}\, \underline{e}_j\,,\ \frac{-\zeta S}{K_j + \zeta^2 M_j}\, \underline{e}_j \right), \tag{4.23}$$

where

$$\mathcal{G}_\zeta(x) = \begin{cases} \dfrac{a}{2\zeta}\, e^{-\zeta |x|/a} & \operatorname{Re}\zeta > 0 \\ -\dfrac{a}{2\zeta}\, e^{\zeta |x|/a} & \operatorname{Re}\zeta < 0 \end{cases} \tag{4.24}$$

$$\mathcal{G}'_\zeta(x) = \frac{d}{dx}\mathcal{G}_\zeta(x) = \begin{cases} -\dfrac{1}{2}\operatorname{sgn}(x)\, e^{-\zeta|x|/a} & \operatorname{Re}\zeta > 0 \\ -\dfrac{1}{2}\operatorname{sgn}(x)\, e^{\zeta|x|/a} & \operatorname{Re}\zeta < 0 \end{cases} \tag{4.25}$$

and $j = 1, \ldots, n$. The deficiency indices of A_0 are (n, n).
Notice that functions G_ζ^j satisfy in the sense of distributions

$$(-\mathbf{L} + \zeta)\, G_\zeta^j(x) = \left(0,\ \frac{1}{\rho_0}\delta_{s_j},\ 0,\ -\frac{S}{M_j} \right) \qquad \zeta \in \mathbb{C}\backslash i\mathbb{R}\,, \tag{4.26}$$

where δ_{s_j} is the Dirac delta centered in s_j.
We indicate with $R(\zeta)$ the resolvent of A

$$R(\zeta) = (-A + \zeta)^{-1} \qquad \zeta \in \rho(A) \tag{4.27}$$

where $\rho(A)$ is the resolvent set of the operator A. Being A a skew-adjoint the adjoint of its resolvent is given by the relation $R(\zeta)^* = -R(-\bar{\zeta})$.
We indicate with A^U a generic skew-adjoint extension of A_0 different from A and with $R^U(\zeta)$ its resolvent, clearly $R^U(\zeta)^* = -R^U(-\bar{\zeta})$. From Krein's formula we obtain

$$R^U(\zeta) = R(\zeta) - \sum_{i,j=1}^n \tilde{\Gamma}(\zeta)_{ij}^{-1} \langle\langle G_{-\bar{\zeta}}^j, \cdot \rangle\rangle G_\zeta^i \tag{4.28}$$

where $\tilde{\Gamma}(\zeta)$ is a matrix defined by

$$\tilde{\Gamma}(\zeta)_{ij} - \tilde{\Gamma}(\xi)_{ij} = -(\zeta - \xi)\langle\langle G^j_{-\bar{\zeta}}, G^i_\xi \rangle\rangle \tag{4.29}$$

and satisfying

$$\tilde{\Gamma}(\zeta)^* = -\tilde{\Gamma}(-\bar{\zeta}) \,, \tag{4.30}$$

where * indicates the Hermitian conjugate.
By direct evaluation one obtains that the more general matrix $\tilde{\Gamma}(\zeta)$ satisfying formula (4.29) is

$$\tilde{\Gamma}(\zeta) = \Gamma(\zeta) + \Theta \tag{4.31}$$

where

$$\Gamma(\zeta)_{ij} := -\zeta \left(\frac{1}{a^2 \rho_0} \mathcal{G}_\zeta(s_i - s_j) + \frac{S\delta_{ij}}{K_j + \zeta^2 M_j} \right) \qquad \zeta \in \mathbb{C} \backslash i\mathbb{R} \tag{4.32}$$

and Θ is a constant skew-adjoint matrix.
Since we are interested only in real skew-adjoint extensions of A_0 we have to restrict the choice of Θ to skew-symmetric matrices. Off diagonal elements of the matrix Θ determine the coupling between the j-th oscillator with the pressure field evaluated in $s_i \neq s_j$, since we are looking for "local" couplings between the acoustic field and the oscillators the only possible choice is $\Theta = O_n$, where O_n is the $n \times n$ matrix with all zero entries. We obtain the following theorem

Theorem 4.1. *The linear operator*

$$\hat{A} : D(\hat{A}) \subset \mathcal{H} \to \mathcal{H} \tag{4.33}$$

$$\begin{aligned} D(\hat{A}) = \{ (p, v, \underline{y}, \underline{z}) \, : \, & p \in L^2(\mathbb{R}) \cap H^1(\mathbb{R} \backslash \mathcal{S}), \, v \in H^1(\mathbb{R}), \, \underline{y} \in \mathbb{C}^n, \, \underline{z} \in \mathbb{C}^n, \\ & p(s_i^+) - p(s_i^-) = \sigma_i, \, v(s_j) = z_j, \, \underline{\sigma} \in \mathbb{C}^n \} \,, \end{aligned} \tag{4.34}$$

$$\begin{aligned} & \hat{A}(p, v, \underline{y}, \underline{z}) := \\ & := \left(-a^2 \rho_0 \frac{dv}{dx}, \, -\frac{1}{\rho_0} \frac{dp_0}{dx}, \, \underline{z}, \, -\sum_{j=1}^n \left(\frac{K_j}{M_j} y_j + \frac{S}{M_j} \sigma_j \right) \underline{e}_j \right) \end{aligned} \tag{4.35}$$

is real and skew-adjoint. Here $p_0 \in \bar{H}^1(\mathbb{R})$,

$$p_0(x) := p(x) - \frac{1}{2} \sum_{j=1}^n \sigma_j \, sgn(x - s_j) \,, \tag{4.36}$$

denotes the regular part of p. *The resolvent of* $\hat{A}$, $\hat{R}(\zeta) = (-\hat{A} + \zeta)^{-1}$, *is given by*

$$\hat{R}(\zeta) = R(\zeta) - \sum_{i,j=1}^n \Gamma(\zeta)^{-1}_{ij} \langle\langle G^j_{-\bar{\zeta}}, \cdot \rangle\rangle G^i_\zeta \qquad \zeta \in \mathbb{C} \backslash i\mathbb{R} \,. \tag{4.37}$$

Proof. By general theorems on self-adjoint extensions of symmetric operators, see e.g. [5] and by $\Gamma(\zeta)^* = -\Gamma(-\bar{\zeta})$, it follows that $\det \Gamma(\zeta) \neq 0$ for any $\zeta \in \mathbb{C} \backslash i\mathbb{R}$ and that $\hat{R}(\zeta)$ satisfies the first resolvent identity

$$(\zeta - \xi) \, \hat{R}(\xi) \hat{R}(\zeta) = \hat{R}(\xi) - \hat{R}(\zeta) \tag{4.38}$$

and

$$\hat{R}(\zeta)^* = -\hat{R}(-\zeta) \tag{4.39}$$

Moreover from (A.12) and (A.13) components of vectors G^j_ζ and functions $\Gamma(\zeta)_{ij}$, $i,j = 1,\dots,n$, are analytic in $\zeta \in \mathbb{C}\backslash i\mathbb{R}$. Therefore

$$\hat{A} := -\hat{R}(\zeta)^{-1} + \zeta \tag{4.40}$$

is well defined on

$$D(\hat{A}) := \mathrm{Ran}(\hat{R}(\zeta))\,. \tag{4.41}$$

By (4.38) such a definition of $\hat{A}$ is ζ-independent. $\hat{A}$ is skew-symmetric by (4.39) and is skew-adjoint since $\mathrm{Ran}(-\hat{A} \pm 1) = \mathcal{H}$ by construction.
Thus $(p, v, \underline{y}, \underline{z}) \in D(\hat{A})$ if and only if

$$p(x) = p_\zeta(x) - \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, (v_\zeta(s_j) - z_{\zeta\, j})\, \mathcal{G}'_\zeta(x - s_i)\,, \tag{4.42}$$

$$v(x) = v_\zeta(x) + \frac{\zeta}{a^2\rho_0} \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, (v_\zeta(s_j) - z_{\zeta\, j})\, \mathcal{G}_\zeta(x - s_i)\,, \tag{4.43}$$

$$\underline{y} = \underline{y}_\zeta - S \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, \frac{v_\zeta(s_j) - z_{\zeta\, j}}{K_i + \zeta^2 M_i}\, \underline{e}_i\,, \tag{4.44}$$

$$\underline{z} = \underline{z}_\zeta - \zeta S \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, \frac{v_\zeta(s_j) - z_{\zeta\, j}}{K_i + \zeta^2 M_i}\, \underline{e}_i\,, \tag{4.45}$$

with $(p_\zeta(x)\,, v_\zeta(x)\,, \underline{y}_\zeta\,, \underline{z}_\zeta) \in D(A)$. Posing

$$\hat{A}(p, v, \underline{y}, \underline{z}) \equiv (\hat{A}_1(p, v, \underline{y}, \underline{z}), \hat{A}_2(p, v, \underline{y}, \underline{z}), \hat{A}_3(p, v, \underline{y}, \underline{z}), \hat{A}_4(p, v, \underline{y}, \underline{z}))\,, \tag{4.46}$$

The action of $\hat{A}$ on $(p, v, \underline{y}, \underline{z})$ is given by

$$[\hat{A}_1(p, v, \underline{y}, \underline{z})](x) = -\, a^2\rho_0 \frac{dv_\zeta}{dx}(x) - \zeta \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, (v_\zeta(s_j) - z_{\zeta\, j}) \mathcal{G}'_\zeta(x - s_i) \tag{4.47}$$

$$[\hat{A}_2(p, v, \underline{y}, \underline{z})](x) = -\, \frac{1}{\rho_0} \frac{dp_\zeta}{dx}(x) + \frac{\zeta^2}{a^2\rho_0} \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, (v_\zeta(s_j) - z_{\zeta\, j}) \mathcal{G}_\zeta(x - s_i) \tag{4.48}$$

$$\hat{A}_3(p, v, \underline{y}, \underline{z}) = \underline{z}_\zeta - \zeta S \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, \frac{v_\zeta(s_j) - z_{\zeta\, j}}{K_i + \zeta^2 M_i}\, \underline{e}_i \tag{4.49}$$

$$\hat{A}_4(p, v, \underline{y}, \underline{z}) = -\sum_{1\le j\le n} \frac{K_j}{M_j}\, y_{\zeta\, j}\, \underline{e}_j - \zeta^2 S \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij}\, \frac{v_\zeta(s_j) - z_{\zeta\, j}}{K_i + \zeta^2 M_i}\, \underline{e}_i\,. \tag{4.50}$$

By the definitions of $D(\hat{A})$ and $\Gamma(\zeta)$ one has

$$\hat{A}_1(p, v, \underline{y}, \underline{z}) = -a^2\rho_0\, \frac{dv}{dx} \tag{4.51}$$

$$\hat{A}_3(p, v, \underline{y}, \underline{z}) = \underline{z} \tag{4.52}$$

and, defining

$$\sigma_i := p(s_i^+) - p(s_i^-) = \sum_{j=1}^{n} (\Gamma(\zeta)^{-1})_{ij} \, (v_\zeta(s_j) - z_{\zeta\, j}) \,, \tag{4.53}$$

formula (4.50) becomes

$$\hat{A}_4(p, v, \underline{y}, \underline{z}) = -\sum_{j=1}^{n} \frac{K_j}{M_j} \, y_{\zeta\, j} \, \underline{e}_j - \zeta^2 S \sum_{i=1}^{n} \frac{\sigma_i}{K_i + \zeta^2 M_i} \, \underline{e}_i = \tag{4.54}$$

$$= -\sum_{j=1}^{n} \left(\frac{K_j}{M_j} \, y_j + \frac{S}{M_j} \, \sigma_j \right) \underline{e}_j \,. \tag{4.55}$$

Then, posing

$$p(x) = p_\zeta(x) - \sum_{j=1}^{n} \sigma_j \, \mathcal{G}'_\zeta(x - s_j) = p_0(x) + \frac{1}{2} \sum_{j=1}^{n} \sigma_j \operatorname{sgn}(x - s_j) \,, \tag{4.56}$$

one obtains

$$[\hat{A}_2(p, v, \underline{y}, \underline{z})](x) =$$

$$= -\frac{1}{\rho_0} \frac{dp_0}{dx}(x) - \sum_{j=1}^{n} \frac{\sigma_j}{\rho_0} \left(\frac{d}{dx} \frac{|x - s_j|}{2(x - s_j)} - \left(-\frac{d^2}{dx^2} + \frac{\zeta^2}{a^2} \right) \mathcal{G}_\zeta(x - y_j) \right) = \tag{4.57}$$

$$= -\frac{1}{\rho_0} \frac{dp_0}{dx} \,. \tag{4.58}$$

Finally

$$v(s_k) = v_\zeta(s_k) - \sum_{i,j=1}^{n} (\Gamma(\zeta)^{-1})_{ij} \, (v_\zeta(s_j) - z_{\zeta\, j}) \left((\Gamma(\zeta))_{ki} + \frac{\zeta S \delta_{ki}}{K_i + \zeta^2 M_i} \right) = \tag{4.59}$$

$$= z_{\zeta\, k} - \zeta S \sum_{j=1}^{n} (\Gamma(\zeta)^{-1})_{kj} \, \frac{v_\zeta(s_k) - z_{\zeta\, k}}{K_k + \zeta^2 M_k} = z_k \,. \tag{4.60}$$

□

By the previous theorem the differential equation

$$\frac{d}{dt} \, (p, v, \underline{y}, \underline{z}) = \hat{A}(p, v, \underline{y}, \underline{z}) \tag{4.61}$$

is equivalent to the system of equations

$$\frac{\partial p}{\partial t} = -a^2 \rho_0 \frac{\partial v}{\partial x} \tag{4.62}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0} \frac{\partial p_0}{\partial x} \equiv -\frac{1}{\rho_0} \left(\frac{\partial p}{\partial x} - \sum_{j=1}^{n} \sigma_j \, \delta_{s_j} \right) \tag{4.63}$$

$$\frac{d\underline{y}}{dt} = \underline{z} \tag{4.64}$$

$$\frac{d\underline{z}}{dt} = -\sum_{j=1}^{n} \left(\frac{K_j}{M_j} \, y_j + \frac{S}{M_j} \, \sigma_j \right) \underline{e}_j \, , \tag{4.65}$$

and the corresponding Cauchy problem generates the strongly continuous unitary group of evolution $\exp t\hat{A}$ on $\mathcal{H}$ which preserves $D(\hat{A})$.
It is worth noting that the only local, real, skew-adjoint extension of A_0 different from the free operator A corresponds to the relevant physical coupling between the pressure field and the oscillators.
The next result will be useful in the spectral analysis of $\hat{A}$.

Lemma 4.1. *The matrix*

$$\Gamma_{\pm}(\lambda)^{-1} := \lim_{\varepsilon \downarrow 0} \Gamma(\lambda \pm \varepsilon)^{-1} \tag{4.66}$$

is well defined for any $\lambda \in i\mathbb{R}\backslash\{0\}$.

Proof. We give the proof only for the matrix $\Gamma_+(\lambda)$, the case $\Gamma_-(\lambda)$ is analogous. Let the matrix $\Gamma_+(\zeta)$ the analytic continuation of $\Gamma(\zeta)$ defined for $\mathrm{Re}\,\zeta > 0$ in (4.32) to $\mathbb{C}\backslash \cup_{j=1}^{n} \{\pm i\sqrt{K_j/M_j}\}$. Suppose that $s_i > s_j$ if $i > j$, then

$$\Gamma_+(\zeta) = -\Pi_{ij}(\zeta) - T_{ij}(\zeta) \tag{4.67}$$

where Π_{ij} is the operator

$$\Pi_{ij} = \left(\underline{\phi}^{-}(\zeta) \otimes \underline{\phi}^{+}(\bar{\zeta}) \right) \tag{4.68}$$

with $\underline{\phi}^{\pm}(\zeta) = \sum_i \frac{e^{\pm \zeta s_i / a}}{\sqrt{2a\rho_0}} \underline{e}_i$. While $T(\zeta)$ is the upper triangular matrix

$$T(\zeta)_{ij} = \begin{cases} \frac{\zeta S \delta_{ij}}{K_i + \zeta^2 M_i} + \frac{\sinh \zeta (s_i - s_j)}{a\rho_0} & i \leq j \\ 0 & i > j \end{cases} \tag{4.69}$$

We use the formula

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{\Pi(\zeta) + T(\zeta)} = -\frac{1}{T(\zeta)} + \frac{1}{T(\zeta)} \Pi(\zeta) \frac{1}{\Pi(\zeta) + T(\zeta)} = \tag{4.70}$$

$$= -\sum_{n=0}^{\infty} \frac{(-1)^n}{T(\zeta)} \left(\Pi(\zeta) \frac{1}{T(\zeta)} \right)^n \tag{4.71}$$

for all ζ for which this series converges.
Matrix $T(\zeta)$ is invertible and its inverse $T(\zeta)^{-1}$ is a lower triangular matrix with $\left(T(\zeta)^{-1}\right)_{ii} = 1/\left(T(\zeta)\right)_{ii}$. The eigenvalues of $T(\zeta)^{-1}$ are $1/\left(T(\zeta)\right)_{ii}$ and we can write

$$T(\zeta)^{-1} = D(\zeta)\tilde{T}(\zeta)^{-1} D(\zeta)^{-1} \tag{4.72}$$

where $D(\zeta)$ is a unitary matrix, analytic for $\zeta \in \mathbb{C}\backslash\{0\}$ and

$$\left(\tilde{T}(\zeta)^{-1}\right)_{ij} = \frac{1}{(T(\zeta))_{ii}}\,\delta_{ij} = \frac{K_i + \zeta^2 M_i}{\zeta S}\,\delta_{ij} \tag{4.73}$$

We obtain for $\Gamma_+(\zeta)^{-1}$ the expression

$$\Gamma_+(\zeta)^{-1} = -D(\zeta)\sum_{n=0}^{\infty}(-1)^n\left(\underline{\psi}(\zeta)\otimes\underline{\chi}(\zeta)\right)^n\tilde{T}(\zeta)^{-1}D(\zeta)^{-1} \tag{4.74}$$

with

$$\left(\underline{\psi}(\zeta)\right)_i = \frac{K_i + \zeta^2 M_i}{\zeta S}\left(D(\zeta)^{-1}\underline{\phi}^-(\zeta)\right)_i \tag{4.75}$$

$$\left(\underline{\chi}(\zeta)\right)_i = \left(D(\zeta)^{-1}\underline{\phi}^+(\bar{\zeta})\right)_i \tag{4.76}$$

Then

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{T(\zeta)}+\sum_{n=0}^{\infty}(-1)^n\left(\langle\underline{\chi}(\zeta),\underline{\psi}(\zeta)\rangle_{\mathbb{C}^n}\right)^n D(\zeta)\underline{\psi}(\zeta)\otimes\underline{\chi}(\zeta)\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}\,, \tag{4.77}$$

if the series converges one obtains

$$\Gamma_+(\zeta)^{-1} = -\frac{1}{T(\zeta)} + \frac{D(\zeta)\underline{\psi}(\zeta)\otimes\underline{\chi}(\zeta)\tilde{T}(\zeta)^{-1}D(\zeta)^{-1}}{1+\langle\underline{\chi}(\zeta),\underline{\psi}(\zeta)\rangle_{\mathbb{C}^n}}\,. \tag{4.78}$$

Consider the scalar product in $\mathbb{C}^n$

$$\left\langle\underline{\chi}(\zeta),\underline{\psi}(\zeta)\right\rangle_{\mathbb{C}^n} = \sum_{i=1}^{n}\overline{\left(D(\zeta)^{-1}\underline{\phi}^+(\bar{\zeta})\right)_i}\,\frac{K_i+\zeta^2 M_i}{\zeta S}\,\left(D(\zeta)^{-1}\underline{\phi}^-(\zeta)\right)_i\,. \tag{4.79}$$

Notice that, for $\lambda \in i\mathbb{R}\backslash\{0\}$, $\left\langle\underline{\chi}(\lambda),\underline{\psi}(\lambda)\right\rangle_{\mathbb{C}^n} \in i\mathbb{R}$ and

$$-i\left\langle\underline{\chi}(\lambda),\underline{\psi}(\lambda)\right\rangle_{\mathbb{C}^n} \to +\infty \quad \text{for } \lambda \to +i\infty \tag{4.80}$$

$$-i\left\langle\underline{\chi}(\lambda),\underline{\psi}(\lambda)\right\rangle_{\mathbb{C}^n} \to -\infty \quad \text{for } \lambda \to i0^+\,. \tag{4.81}$$

Then there exists at least one point $\lambda \in i\mathbb{R}$ in which $\langle\underline{\chi}(\lambda),\underline{\psi}(\lambda)\rangle_{\mathbb{C}^n} = 0$. In a neighborhood of this point the series converges and defines an analytic function. By (4.78) and (4.79) it is clear that $\Gamma_+(\zeta)^{-1}$ exists for any $\zeta \in \mathbb{C}\backslash\{0\}$. The same relations show that one can put $\Gamma_+(\zeta)^{-1} := 0$ if $\zeta = i\sqrt{K_j/M_j}$, $j = 1,\ldots,n$. □

The following theorem completely characterizes the spectrum of $\hat{A}$.

Theorem 4.2. *The essential spectrum of $\hat{A}$ is purely absolutely continuous and*

$$\sigma_{ess}(\hat{A}) = \sigma_{ac}(\hat{A}) = i\mathbb{R}\,, \qquad \sigma_{pp}(\hat{A}) = \{0\}\,. \tag{4.82}$$

Any vector of the kind

$$\left(\frac{1}{2}\sum_{j=1}^{n}\sigma_j\,sgn(x-s_j),\,0,\,-\sum_{j=1}^{n}\frac{S}{K_j}\,\sigma_j\,\underline{e}_j,\,\underline{0}\right)\,, \tag{4.83}$$

with

$$\sum_{j=1}^{n} \sigma_j = 0\,, \tag{4.84}$$

is an eigenvector corresponding to the $(n-1)$-fold degenerate eigenvalue $\lambda = 0$. The generalized eigenfunctions $\hat{\Phi}^{\pm}(\lambda)$ corresponding to the point of the absolutely continuous spectrum relative to right $(+)$ and left $(-)$ incidence are given by

$$\hat{\Phi}^{\pm}(\lambda, x) = \left(\hat{\phi}_p^{\pm}(\lambda, x), \hat{\phi}_v^{\pm}(\lambda, x), \hat{\phi}_{\underline{y}}^{\pm}(\lambda), \hat{\phi}_{\underline{z}}^{\pm}(\lambda)\right) \qquad \lambda \in i\mathbb{R} \tag{4.85}$$

$$\hat{\phi}_p^{\pm}(\lambda, x) = Ce^{\pm\lambda x/a} \mp \frac{C}{2a\rho_0} \sum_{i,j=1}^{n} (\Gamma_+(\lambda)^{-1})_{ij} e^{\pm\lambda s_j/a} sgn(x - s_i) e^{-\lambda|x-s_i|/a} \tag{4.86}$$

$$\hat{\phi}_v^{\pm}(\lambda, x) = \mp C\frac{e^{\pm\lambda x/a}}{a\rho_0} \mp \frac{C}{2a^2\rho_0^2} \sum_{i,j=1}^{n} (\Gamma_+(\lambda)^{-1})_{ij} e^{\pm\lambda s_j/a} e^{-\lambda|x-s_i|/a} \tag{4.87}$$

$$\hat{\phi}_{\underline{y}}^{\pm}(\lambda) = \pm\frac{SC}{a\rho_0} \sum_{i,j=1}^{n} (\Gamma_+(\lambda)^{-1})_{ij} \frac{e^{\pm\lambda s_j/a}}{K_i + \lambda^2 M_i} \underline{e}_i \tag{4.88}$$

$$\hat{\phi}_{\underline{z}}^{\pm}(\lambda) = \pm\frac{\lambda SC}{a\rho_0} \sum_{1\le i,j\le n} (\Gamma_+(\lambda)^{-1})_{ij} \frac{e^{\pm\lambda s_j/a}}{K_i + \lambda^2 M_i} \underline{e}_i \tag{4.89}$$

with $C = \sqrt{a\rho_0/(4\pi)}$.

Proof. For $\zeta \in \rho(A)\cap\rho(\hat{A})$, $(-\hat{A}+\zeta)^{-1} - (-A+\zeta)^{-1}$ is of finite rank, then from Weyl's criterion (see e.g. [41] Theorem XIII.14) one has $\sigma_{ess}(\hat{A}) = \sigma_{ess}(A) = i\mathbb{R}$. Moreover, by Birman-Kato invariance principle, the wave operators $\Omega_{\pm}(\hat{A}, A)$ exist and are complete (see e.g. [42], Corollary 2 to Theorem XI.11). Thus $\sigma_{ac}(\hat{A}) = \sigma_{ac}(A)$.
Let $\hat{\mu}_{\Psi}^{sc}$ be the singular continuous part of the spectral measure on $i\mathbb{R}$ corresponding to $\hat{A}$ and Ψ. Since $\|\breve{G}(\zeta)\Psi\| < \infty$ for all $\zeta \in \mathbb{C}\backslash\sigma_{pp}(A)$ and for all $\Psi \in D$,

$$D := \left\{\Psi \equiv (p, v, \underline{y}, \underline{z}) \,:\, p \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})\,, \quad v \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})\right\}\,, \tag{4.90}$$

by Lemma 4.1 and [41], Theorem XIII.19, one has supp $\hat{\mu}_{\Psi}^{sc} \subseteq \{0\} \cup \sigma_{pp}(A)$ i.e. supp $\hat{\mu}_{\Psi}^{sc} = \emptyset$ since $\hat{\mu}_{\Psi}^{sc}$ has no atoms by its definition. Since D is dense this gives $\sigma_{sc}(\hat{A}) = \emptyset$.
One can check that any vector Ψ of the kind (4.83) is in the domain of $\hat{A}$ and solves the equation $\hat{A}\Psi = 0$. The degeneration of eigenvalue $\{0\}$ follows from condition (4.84).
Suppose now $\lambda \in i\mathbb{R}\backslash\{0\}$ and consider the equation $\hat{A}\Psi = \lambda\Psi$. This produces, if $\Psi \equiv (p, v, \underline{y}, \underline{z})$, the equation

$$v'' - \frac{\lambda^2}{a^2}\, v = -\frac{\lambda}{a^2\rho_0} \sum_{j=1}^{n} \sigma_j \delta_{s_j}\,, \tag{4.91}$$

with $\sigma_i \in \mathbb{C}$, $i = 1, \ldots, n$, which has no square integrable solution.

The expression for the generalized eigenfunctions is a consequence of the Stone's formula (see e.g. [39], Theorem VII.13) which gives the generalized expansion formula

$$\Psi = \mathrm{s}\text{-}\lim_{a\downarrow -\infty,\, b\uparrow\infty} \mathrm{s}\text{-}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi}\int_a^b [\hat{R}(\lambda+\varepsilon) - \hat{R}(\lambda-\varepsilon)]\Psi\, d\lambda\,. \tag{4.92}$$

□

In the following lemma the asymptotic behavior of the oscillations of the thin walls is characterized.

Lemma 4.2. *Given Ψ_0 orthogonal to the eigenspace relative to eigenvalue zero, let us denote by $\big(\underline{y}(t), \underline{z}(t)\big)$ the projection onto $\mathbb{C}^n \oplus \mathbb{C}^n$ of $e^{t\hat{A}}\Psi_0$. Then*

$$\lim_{|t|\to\infty} \|\underline{y}(t)\|_{\mathbb{C}^n} = 0 \quad \textit{and} \quad \lim_{|t|\to\infty} \|\underline{z}(t)\|_{\mathbb{C}^n} = 0\,.$$

Proof. Let $\hat{P}(dk)$ be the projection-valued measure corresponding to the self-adjoint operator $-i\hat{A}$. Since Ψ_0 is in the absolutely continuous subspace, for any Ψ the bounded complex measure $\langle\langle\Psi, \hat{P}(dk)\Psi_0\rangle\rangle$ is absolutely continuous with respect to Lebesgue measure and hence its density belongs to $L^1(\mathbb{R})$. Thus, by the spectral theorem and Riemann-Lebesgue lemma,

$$\lim_{|t|\to\infty} \langle\langle\Psi, e^{t\hat{A}}\Psi_0\rangle\rangle = \lim_{|t|\to\infty} \int_{\mathbb{R}} e^{-itk}\, \langle\langle\Psi, \hat{P}(dk)\Psi_0\rangle\rangle = 0\,. \tag{4.93}$$

By taking $\Psi = (0, 0, \underline{e}_i, \underline{0})$ and $\Psi = (0, 0, \underline{0}, \underline{e}_i)$, $i = 1, \ldots, n$, one then obtains

$$\lim_{|t|\to\infty} y_i(t) = 0 \quad \text{and} \quad \lim_{|t|\to\infty} z_i(t) = 0\,. \tag{4.94}$$

□

In order to obtain more precise estimate on the asymptotic behavior of solutions of equation (4.61), for particular initial conditions, a detailed analysis of $\Gamma(\lambda)^{-1}$ is required. For example in specific cases one can prove existence of frequencies which are totally transmitted by the array of oscillators.
In [16] one can find a different derivation of operator $\hat{A}$ obtained by using the technique developed by A. Posilicano in [37] (also see the appendix in [38] for a compact review).

4.3 Kronig-Penney model in acoustics

It is possible to extend the previous construction to the case of an array of infinitely many oscillators. We prove that in the case of a periodical array of identical oscillators the energy spectrum shows a band structure.
The construction of $\hat{A}$ when $\mathcal{S} = \{s_1, s_2, \ldots\}$ is a denumerable set such that

$$d := \inf_{i\neq j} |s_i - s_j| > 0 \quad i, j \in \mathbb{N}. \tag{4.95}$$

follows closely what was done in [9]. We state the final result, for more details the reader can refer to [16]

Theorem 4.3. *Let* $\{K_j\}_1^\infty$ $\{M_j\}_1^\infty$, $K_j > 0$, $M_j > 0$ *be in* ℓ^∞ *and suppose that* $\{K_j/M_j\}_1^\infty$ *and* $\{1/M_j\}_1^\infty$ *are in* ℓ^∞ *too. The linear operator*

$$\hat{A} : D(\hat{A}) \subset L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \ell^2 \oplus \ell^2 \to L^2(\mathbb{R}) \oplus L^2(\mathbb{R}) \oplus \ell^2 \oplus \ell^2 \,, \qquad (4.96)$$

$$\begin{aligned} D(\hat{A}) = \{(p, v, \underline{y}, \underline{z}) \,:\, & p \in L^2(\mathbb{R}) \cap H^1(\mathbb{R}\backslash\mathcal{S}),\, v \in H^1(\mathbb{R}),\ \underline{y} \in \ell^2,\, \underline{z} \in \ell^2, \\ & p(s_i^+) - p(s_i^-) = \sigma_i,\ v(s_j) = z_j,\ \underline{\sigma} \in \ell^2\} \,, \end{aligned} \qquad (4.97)$$

$$\begin{aligned} & \hat{A}(p, v, \underline{y}, \underline{z}) := \\ & := \left(-a^2 \rho_0 \frac{dv}{dx}, -\frac{1}{\rho_0} \frac{dp_0}{dx}, \underline{z}, -\sum_{j=1}^{\infty} \left(\frac{K_j}{M_j}\, y_j + \frac{S}{M_j}\, \sigma_j \right) \underline{e}_j \right) \end{aligned} \qquad (4.98)$$

is real and skew-adjoint. Here $p_0 \in \bar{H}^1(\mathbb{R})$,

$$p_0(x) := p(x) - \frac{1}{2} \sum_{j=1}^{\infty} \sigma_j \, sgn(x - s_j) \,, \qquad (4.99)$$

denotes the regular part of p. *The resolvent of* $\hat{A}$ *is given by*

$$\hat{R}(\zeta) = R(\zeta) - \sum_{i,j=1}^{\infty} \Gamma(\zeta)_{ij}^{-1} \, \langle\langle G^j_{-\bar{\zeta}}, \cdot \rangle\rangle G^i_\zeta \qquad \zeta \in \mathbb{C}\backslash i\mathbb{R} \,. \qquad (4.100)$$

Now we can proceed to the study of a periodic system. We use the same notation of [8].
In this case $\mathcal{S}$ will be the "Bravais" lattice,

$$\mathcal{S} = \{nL : n \in \mathbb{Z}\} \,, \quad L > 0 \,, \qquad (4.101)$$

and $\hat{\mathcal{S}}$ the "Brillouin" zone,

$$\hat{\mathcal{S}} = \left[-\frac{b}{2}, \frac{b}{2} \right) \,, \quad b = \frac{2\pi}{L} \,. \qquad (4.102)$$

We consider a Hilbert space $\mathcal{H}$ on $L^2 \oplus L^2 \oplus \ell^2 \oplus \ell^2$ in which the scalar product is defined by

$$\frac{1}{a^2 \rho_0}(p_1, p_2) + \rho_0(v_1, v_2) + \frac{K}{S}(\underline{y}_1, \underline{y}_2) + \frac{M}{S})(\underline{z}_1, \underline{z}_2) \qquad (4.103)$$

where $(\cdot, \cdot)$ represents either the usual scalar product in L^2, when concerning pressure and velocity fields, or the usual scalar product in ℓ^2, for $\underline{y}$ and $\underline{z}$.
M, K and S are positive constants representing the mass of oscillating walls, the elastic constant of the springs and the area of the transversal section of the pipe.
The Hilbert space $\mathcal{H}$ can be decomposed as

$$\mathcal{H} = \tilde{\mathscr{W}}^{-1} \tilde{\mathcal{H}}(\hat{\mathcal{S}}, b^{-1} d\theta; L^2([-L/2, L/2)) \oplus L^2([-L/2, L/2)) \oplus \mathbb{C} \oplus \mathbb{C}) \qquad (4.104)$$

$$= \tilde{\mathscr{W}}^{-1} \int_{[-b/2, b/2)}^{\oplus} \frac{d\theta}{b} \left(L^2([-L/2, L/2)) \oplus L^2([-L/2, L/2)) \oplus \mathbb{C} \oplus \mathbb{C} \right) \qquad (4.105)$$

where

$$\tilde{\mathscr{W}} : \mathcal{H} \to \tilde{\mathcal{H}}(\hat{\mathcal{S}}, b^{-1}d\theta; L^2([-L/2, L/2)) \oplus L^2([-L/2, L/2)) \oplus \mathbb{C} \oplus \mathbb{C}) \quad (4.106)$$

$$\tilde{\mathscr{W}}(p, v, \underline{y}, \underline{z}) \equiv \Big((\tilde{W}p)(\theta, \nu), (\tilde{W}v)(\theta, \nu), (\tilde{W}\underline{y})(\theta), (\tilde{W}\underline{z})(\theta) \Big) \quad (4.107)$$

$$(\tilde{W}p)(\theta, \nu) \equiv \tilde{p}(\theta, \nu) = \sum_{n \in \mathbb{Z}} e^{in\theta L} p(\nu + nL) \quad (4.108)$$

$$(\tilde{W}v)(\theta, \nu) \equiv \tilde{v}(\theta, \nu) = \sum_{n \in \mathbb{Z}} e^{in\theta L} v(\nu + nL) \quad (4.109)$$

$$(\tilde{W}\underline{y})(\theta) \equiv \tilde{y}(\theta) = \sum_{n \in \mathbb{Z}} e^{in\theta L} y_n \quad (4.110)$$

$$(\tilde{W}\underline{z})(\theta) \equiv \tilde{z}(\theta) = \sum_{n \in \mathbb{Z}} e^{in\theta L} z_n \qquad \nu \in [-L/2, L/2)\,, \quad \theta \in [-b/2, b/2) \quad (4.111)$$

and

$$\tilde{\mathscr{W}}^{-1} : \tilde{\mathcal{H}}(\hat{\mathcal{S}}, b^{-1}d\theta; L^2([-L/2, L/2)) \oplus L^2([-L/2, L/2)) \oplus \mathbb{C} \oplus \mathbb{C}) \to \mathcal{H} \quad (4.112)$$

$$\tilde{\mathscr{W}}^{-1}(\tilde{p}, \tilde{v}, \underline{\tilde{y}}, \underline{\tilde{z}}) \equiv$$
$$\equiv \Big((\tilde{W}^{-1}\tilde{p})(\nu + nL), (\tilde{W}^{-1}\tilde{v})(\nu + nL), \{(\tilde{W}^{-1}\tilde{y})_n\}, \{(\tilde{W}^{-1}\tilde{z})_n\} \Big) \quad (4.113)$$

$$(\tilde{W}^{-1}\tilde{p})(\nu + nL) = b^{-1} \int_{-b/2}^{b/2} d\theta e^{-in\theta L} \tilde{p}(\theta, \nu) \quad (4.114)$$

$$(\tilde{W}^{-1}\tilde{v})(\nu + nL) = b^{-1} \int_{-b/2}^{b/2} d\theta e^{-in\theta L} \tilde{v}(\theta, \nu) \quad (4.115)$$

$$(\tilde{W}^{-1}\tilde{y})_n = b^{-1} \int_{-b/2}^{b/2} d\theta e^{-in\theta L} \tilde{y}(\theta) \quad (4.116)$$

$$(\tilde{W}^{-1}\tilde{z})_n = b^{-1} \int_{-b/2}^{b/2} d\theta e^{-in\theta L} \tilde{z}(\theta) \qquad \nu \in [-L/2, L/2)\,, \quad n \in \mathbb{Z}\,. \quad (4.117)$$

The scalar product in $L^2([-L/2, L/2)) \oplus L^2([-L/2, L/2)) \oplus \mathbb{C} \oplus \mathbb{C}$ is defined by

$$\frac{1}{a^2\rho_0}(\tilde{p}_1, \tilde{p}_2)_{L/2} + \rho_0(\tilde{v}_1, \tilde{v}_2)_{L/2} + \frac{K}{S}\bar{\tilde{y}}_1\tilde{y}_2 + \frac{M}{S}\bar{\tilde{z}}_1\tilde{z}_2 \quad (4.118)$$

where $(\cdot, \cdot)_{L/2}$ indicates the usual scalar product in $L^2([-L/2, L/2))$.
From Theorem 4.3 we obtain the following

Corollary 4.3.1. *The linear operator*

$$\hat{A} : D(\hat{A}) \subset \mathcal{H} \to \mathcal{H} \quad (4.119)$$

$$D(\hat{A}) = \Big\{ (p, v, \underline{y}, \underline{z}) \, : p \in L^2(\mathbb{R}) \cap H^1(\mathbb{R} \backslash \mathcal{S})\,,\ v \in H^1(\mathbb{R})\,, \underline{y} \in \ell^2\,,\ \underline{z} \in \ell^2\,,$$
$$p(nL^+) - p(nL^-) = \sigma_n\,, v(nL) = z_n \ \forall n \in \mathbb{Z}\,,\ \underline{\sigma} \in \ell^2 \Big\} \quad (4.120)$$

$$\hat{A}(p,v,\underline{y},\underline{z}) := \left(-a^2\rho_0\frac{dv}{dx}, -\frac{1}{\rho_0}\frac{dp_0}{dx}, \underline{z}, -\frac{K}{M}\underline{y} - \frac{S}{M}\underline{\sigma}\right), \tag{4.121}$$

where the regular part of $p(x)$*, denoted with* $p_0 \in \bar{H}^1(\mathbb{R})$*, is*

$$p_0(x) = p(x) - \frac{1}{2}\sum_{n\in\mathbb{Z}} \sigma_n\, sgn(x-nL)\,, \tag{4.122}$$

is real and skew-adjoint.

We want to study the spectral structure of $\hat{A}$. To this aim we introduce the family of operators $\hat{A}(\theta)$

$$\begin{aligned}\hat{A}(\theta) : D(\hat{A}(\theta)) \subset L^2((-L/2,L/2)) \oplus L^2((-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C} \\ \to L^2((-L/2,L/2)) \oplus L^2((-L/2,L/2)) \oplus \mathbb{C} \oplus \mathbb{C}\end{aligned} \tag{4.123}$$

$$\begin{aligned} D(\hat{A}(\theta)) = \Bigg\{ &(\tilde{p}(\theta), \tilde{v}(\theta), \tilde{y}(\theta), \tilde{z}(\theta)) \; : \\ &\tilde{p}(\theta) \in H^1((-L/2,L/2)\backslash\{0\})\,,\ \tilde{v}(\theta) \in H^1((-L/2,L/2))\,, \\ &\tilde{y}(\theta) \in \mathbb{C}\,,\ \tilde{z}(\theta) \in \mathbb{C} \\ &\tilde{p}(\theta,0^+) - \tilde{p}(\theta,0^-) = \tilde{\sigma}(\theta)\,, \\ &\tilde{v}(\theta,0) = \tilde{z}(\theta)\,,\ \tilde{\sigma}(\theta) \in \mathbb{C}\,, \\ &\tilde{p}\left(\theta, -\frac{L^+}{2}\right) = e^{i\theta L}\tilde{p}\left(\theta, \frac{L^-}{2}\right), \\ &\tilde{v}\left(\theta, -\frac{L^+}{2}\right) = e^{i\theta L}\tilde{v}\left(\theta, \frac{L^-}{2}\right)\Bigg\}; \quad \forall\theta \in \left[-\frac{b}{2}, \frac{b}{2}\right) \end{aligned} \tag{4.124}$$

$$\begin{aligned}&\hat{A}(\theta)(\tilde{p}(\theta), \tilde{v}(\theta), \tilde{y}(\theta), \tilde{z}(\theta)) := \\ &\quad := \left(-a^2\rho_0\frac{d\tilde{v}(\theta)}{d\nu}, -\frac{1}{\rho_0}\frac{d\tilde{p}_0(\theta)}{d\nu}, \tilde{z}(\theta), -\frac{K}{M}\tilde{y}(\theta) - \frac{S}{M}\tilde{\sigma}(\theta)\right)\end{aligned} \tag{4.125}$$

where $\tilde{p}_0(\theta) \in H^1(\mathbb{R})$ is the regular part of $\tilde{p}(\theta)$

$$\tilde{p}_0(\theta,\nu) = \tilde{p}(\theta,\nu) - \frac{1}{2}\tilde{\sigma}(\theta)\,\mathrm{sgn}(\nu)\,. \tag{4.126}$$

Boundary conditions for $\tilde{p}(\theta,\nu)$ and $\tilde{v}(\theta,\nu)$ in $\nu = 0$ and $\nu = \pm L/2$ are such that all operators in this family are skew-adjoint with respect to the scalar product (4.118).
The operator $\hat{A}$ is related to $\hat{A}(\theta)$ by the relation (see [8])

$$\tilde{\mathscr{W}}\hat{A}\tilde{\mathscr{W}}^{-1} = \int_{[-b/2,b/2)}^{\oplus} \frac{d\theta}{b}\hat{A}(\theta)\,. \tag{4.127}$$

The spectrum of $\hat{A}(\theta)$ is described by the following

Theorem 4.4. *Let* $\theta \in [-b/2, b/2)$ *then the spectrum of* $\hat{A}(\theta)$ *is purely discrete, in particular its eigenvalues* $E_n(\theta)$ *are given by*

$$E_n(\theta) = \lambda_n(\theta) = 2i\xi_n(\theta)\frac{a}{L}\,; \quad n \in \mathbb{Z}\,,\ \xi_n(\theta) \in \mathbb{R} \tag{4.128}$$

where $\xi_n(\theta)$ *are the real solutions of*

$$\sin\xi\left[\sin\xi - F(\xi)\cos\xi\right]\cos^2\frac{\theta L}{2} = \cos\xi\left[\cos\xi + F(\xi)\sin\xi\right]\sin^2\frac{\theta L}{2} \tag{4.129}$$

$$F(\xi) = \frac{M}{M_g}\left(\pi^2\frac{\omega_o^2}{\omega_g^2}\frac{1}{\xi} - \xi\right)\ ; \quad M_g = \rho_0 SL,\ \omega_o^2 = \frac{K}{M},\ \omega_g = 2\pi\frac{a}{L}. \tag{4.130}$$

The corresponding eigenfunctions are

$$\Phi_n(\theta, x) = (\tilde{p}_n(\theta,\nu), \tilde{v}_n(\theta,\nu), \tilde{y}_n(\theta), \tilde{z}_n(\theta))\ ; \quad n\in\mathbb{Z},\ \theta\in[-b/2, b/2) \tag{4.131}$$

$$\begin{aligned}\tilde{p}_n(\theta,\nu) =& C_n\Bigg[\left(\sin\left(\xi_n - \frac{\theta L}{2}\right) - F(\xi_n)\cos\left(\xi_n - \frac{\theta L}{2}\right)\right)\cos\frac{2\xi_n}{L}\nu + \\ & - i\sin\left(\xi_n - \frac{\theta L}{2}\right)\left(\sin\frac{2\xi_n}{L}\nu - F(\xi_n)\frac{|\nu|}{\nu}\cos\frac{2\xi_n}{L}\nu\right)\Bigg] \end{aligned}\tag{4.132}$$

$$\begin{aligned}\tilde{v}_n(\theta,\nu) =& -\frac{iC_n}{a\rho_0}\Bigg[\left(\sin\left(\xi_n - \frac{\theta L}{2}\right) - F(\xi_n)\cos\left(\xi_n - \frac{\theta L}{2}\right)\right)\sin\frac{2\xi_n}{L}\nu + \\ & + i\sin\left(\xi_n - \frac{\theta L}{2}\right)\left(\cos\frac{2\xi_n}{L}\nu + F(\xi_n)\sin\frac{2\xi_n}{L}|\nu|\right)\Bigg] \end{aligned}\tag{4.133}$$

$$\tilde{y}_n(\theta) = -i\frac{C_n L}{a^2\rho_0\xi_n}\sin\left(\xi_n - \frac{\theta L}{2}\right) \tag{4.134}$$

$$\tilde{z}_n(\theta) = \frac{C_n}{a\rho_0}\sin\left(\xi_n - \frac{\theta L}{2}\right) \tag{4.135}$$

For $\theta\in[-b/2, b/2)$ *zero is an eigenvalue with eigenfunction*

$$\Psi_0 = \left(C_0\left(\cos\frac{\theta L}{2} - i\sin\frac{\theta L}{2}sgn(\nu)\right), 0, 2iC_0\frac{S}{K}\sin\frac{\theta L}{2}, 0\right) \tag{4.136}$$

Moreover the following chain of inequalities holds

$$\begin{aligned}&0 < E_1(0) < E_1(-b/2) \le E_2(-b/2) < E_2(0) \le E_3(0) < E_3(-b/2) \le \\ &\le E_4(-b/2) < E_4(0) \le E_5(0) < E_4(-b/2) \le E_5(-b/2) < \dots\end{aligned}\tag{4.137}$$

In general eigenvalues $E_n(\theta)$ *are all distinct and non degenerate. If* $\omega_o/\omega_g = n/2$ *with* $n\in\mathbb{N}$ *there is just one two fold degenerate eigenvalue equal to* $n\pi/2$*, such eigenvalue corresponds to* $\theta = 0$ *for* n *even and to* $|\theta| = b/2$ *for* n *odd.*
If $E(\theta)$ *is an eigenvalue then* $-E(\theta)$ *is an eigenvalue.*
Given $\theta\in[-b/2, b/2)$ *the following relation holds*

$$E_n(-\theta) = E_n(\theta)\,. \tag{4.138}$$

Proof. Eigenvalues and eigenfunctions (4.128)-(4.136) are given by direct calculation. We solve the system of equations

$$\hat{A}(\theta)(\tilde{p}(\theta), \tilde{v}(\theta), \tilde{y}(\theta), \tilde{z}(\theta)) = \lambda(\tilde{p}(\theta), \tilde{v}(\theta), \tilde{y}(\theta), \tilde{z}(\theta)) \qquad \lambda\in i\mathbb{R} \tag{4.139}$$

with the condition $\tilde{v}(\theta, 0) = \tilde{z}(\theta)$, the solution reads

$$\tilde{p}(\theta, \nu) = C(\xi) \cos \frac{2\xi\nu}{L} + D(\xi) \left[\sin \frac{2\xi\nu}{L} - F(\xi) \mathrm{sgn}(\nu) \cos \frac{2\xi\nu}{L} \right] \tag{4.140}$$

$$\tilde{v}(\theta, \nu) = \frac{C(\xi)}{ia\rho_0} \sin \frac{2\xi\nu}{L} - \frac{D(\xi)}{ia\rho_0} \left[\cos \frac{2\xi\nu}{L} + F(\xi) \sin \frac{2\xi|\nu|}{L} \right] \tag{4.141}$$

where $\xi = -iL\lambda/(2a) \in \mathbb{R}$, $C(\xi)$ and $D(\xi)$ are two unknown functions of ξ. To determine $C(\xi)$ and $D(\xi)$ we have to take into account the boundary conditions

$$\begin{cases} \tilde{p}\left(\theta, -\frac{L^+}{2}\right) = e^{i\theta L} \tilde{p}\left(\theta, \frac{L^-}{2}\right) \\ \tilde{v}\left(\theta, -\frac{L^+}{2}\right) = e^{i\theta L} \tilde{v}\left(\theta, \frac{L^-}{2}\right) \end{cases} \tag{4.142}$$

This system has only the trivial solution $C(\xi) = 0$ and $D(\xi) = 0$ unless we consider the values of ξ for which the determinant of the matrix of the coefficients of the system is zero, this condition implies equation (4.129) for the eigenvalues. For ξ satisfying condition (4.129) the solutions of the system of dependent equations (4.142) give the eigenfunctions.
For $\theta = 0$ and $\theta = -b/2$ relation (4.129) becomes

$$\tan \xi = 0 \quad \text{or} \quad \tan \xi = F(\xi) = \frac{M}{M_g} \left(\pi^2 \frac{\omega_o^2}{\omega_g^2} \frac{1}{\xi} - \xi \right) \quad ; \quad \theta = 0 \tag{4.143}$$

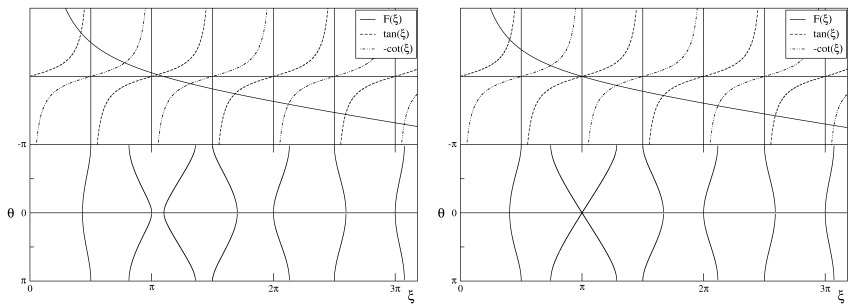
$$\cot \xi = 0 \quad \text{or} \quad -\cot \xi = F(\xi) = \frac{M}{M_g} \left(\pi^2 \frac{\omega_o^2}{\omega_g^2} \frac{1}{\xi} - \xi \right) \quad ; \quad \theta = -b/2 \tag{4.144}$$

Graphic solutions of the transcendental equations (4.143) and (4.144) are given in the upper part of figures 4.1(a) and 4.1(b). The chain of inequalities (4.137) follows by the monotone behavior of $F(\xi)$.
Degeneration of eigenvalues for $\omega_o/\omega_g = n/2$, the fact that $-E(\theta)$ is an eigenvalue if $E(\theta)$ is an eigenvalue and relation (4.138) follow directly by equation (4.129) and by $F(\xi) = -F(-\xi)$. □

One can show that there is a band structure writing equation (4.129) as

$$\tan^2 \frac{\theta L}{2} = \tan \xi \left[\frac{\tan \xi - F(\xi)}{1 + F(\xi) \tan \xi} \right] \tag{4.145}$$

It is possible to find solutions of equation (4.145) only for values of ξ such that the r.h.s. is positive. In the lower part of figures 4.1(b) and 4.1(a) the resulting band structure is shown. The figures clearly show that the width of the gaps is connected to the structure of the spectrum. In particular figure 4.1(b) shows that when there is a degenerate eigenvalue, $\omega_o/\omega_g = n\pi/2$ with $n \in \mathbb{N}$, a gap disappears because of the overlapping of two bands.
The bandwidth increases, when the ratio M/M_g decreases.



(a) With non degenerate eigenvalues. $M/M_g = 0.5$, $\omega_o/\omega_g = 1.2$

(b) With one degenerate eigenvalue. $M/M_g = 0.5$, $\omega_o/\omega_g = 1$

Figure 4.1: The upper part of figures shows the graphical solution of equations (4.143) and (4.144). The lower part shows the band structure due to equation (4.145)

4.4 Homogenization

We derive a limit equation for the velocity field when infinite oscillators are distribuited with uniform density on a segment of lenght L of the x-axis.
As first step we find a closed equation for the velocity field when the number of oscillators is N. Consider the system of equations

$$\frac{\partial p}{\partial t} = -a^2 \rho_0 \frac{\partial v}{\partial x} \tag{4.146}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{\rho_0}\frac{\partial p_0}{\partial x} = -\frac{1}{\rho_0}\left(\frac{\partial p}{\partial x} - \sum_{j=1}^{N} \sigma_j \, \delta_{s_j}\right) \tag{4.147}$$

$$\frac{dy_j}{dt} = z_j \tag{4.148}$$

$$\frac{dz_j}{dt} = -\left(\frac{K_j}{M_j} y_j + \frac{S}{M_j}\sigma_j\right) \tag{4.149}$$

with

$$p(x) = p_0(x) + \frac{1}{2}\sum_{j=1}^{N} \sigma_j \, \mathrm{sgn}(x - s_j)\,. \tag{4.150}$$

From equation (4.146) we obtain

$$\frac{\partial p_0}{\partial t} + \frac{1}{2}\sum_{j=1}^{N} \dot{\sigma}_j \, \mathrm{sgn}(x - s_j) = -a^2 \rho_0 \frac{\partial v}{\partial x} \tag{4.151}$$

taking the derivative of (4.151) with respect to x and the derivative of (4.147) with respect to t

$$\frac{\partial^2 p_0}{\partial x \partial t} + \sum_{j=1}^{N} \dot{\sigma}_j \, \delta_{s_j} = -a^2 \rho_0 \frac{\partial^2 v}{\partial x^2} \tag{4.152}$$

$$\frac{\partial^2 v}{\partial t^2} = -\frac{1}{\rho_0} \frac{\partial^2 p_0}{\partial t \partial x} \tag{4.153}$$

The function p_0 is the regular part of p, then we can assume that

$$\frac{\partial^2 p_0}{\partial x \partial t} = \frac{\partial^2 p_0}{\partial t \partial x} \tag{4.154}$$

we obtain the following equation for v

$$\frac{1}{a^2} \frac{\partial^2 v}{\partial t^2} - \frac{\partial^2 v}{\partial x^2} = \frac{1}{a^2 \rho_0} \sum_{j=1}^{N} \dot{\sigma}_j \, \delta_{s_j} \tag{4.155}$$

Taking the derivative of (4.148) and (4.149) with respect to t

$$\frac{d^2 z_j}{dt^2} = -\left(\frac{K_j}{M_j} z_j + \frac{S}{M_j} \dot{\sigma}_j \right) \tag{4.156}$$

and noticing that

$$z_j = v(s_j) \text{ and } \quad \frac{d^2 z_j}{dt^2} = \frac{\partial^2 v}{\partial t^2}\Big|_{x=s_j} \tag{4.157}$$

from (4.156)

$$\dot{\sigma}_j = -\frac{M_j}{S} \frac{\partial^2 v}{\partial t^2}\Big|_{x=s_j} - \frac{K_j}{S} v(s_j) \,, \tag{4.158}$$

we obtain the closed equation for v

$$\frac{1}{a^2} \frac{\partial^2 v}{\partial t^2} - \frac{\partial^2 v}{\partial x^2} = -\frac{1}{a^2 \rho_0} \sum_{j=1}^{N} \left(\frac{M_j}{S} \frac{\partial^2 v}{\partial t^2}\Big|_{x=s_j} + \frac{K_j}{S} v(s_j) \right) \delta_{s_j} \tag{4.159}$$

Define two positive functions $\rho_M(x)$ and $\rho_K(x)$ such that ρ_M, $\rho_K \in L^1(\mathbb{R})$ and

$$M_j = \frac{L}{N} \rho_M(s_j) \text{ and } K_j = \frac{L}{N} \rho_K(s_j) \tag{4.160}$$

where $L = \max_{i,j}(|s_i - s_j|)$. We suppose to increase L by taking L fixed, the following limits hold

$$\begin{aligned} &\sum_{j=1}^{N} M_j \frac{\partial^2 v}{\partial t^2}\Big|_{x=s_j} \delta_{s_j} = \frac{L}{N} \sum_{j=1}^{N} \rho_M(s_j) \frac{\partial^2 v}{\partial t^2}\Big|_{x=s_j} \delta_{s_j} \to \\ &\to \int \rho_M(x') \frac{\partial^2 v(x')}{\partial t^2} \delta(x - x') dx' = \rho_M(x) \frac{\partial^2 v(x)}{\partial t^2} \quad N \to \infty \end{aligned} \tag{4.161}$$

$$\begin{aligned} &\sum_{j=1}^{N} K_j v(s_j) \delta_{s_j} = \frac{L}{N} \sum_{j=1}^{N} \rho_K(s_j) v(s_j) \delta_{s_j} \to \\ &\to \int \rho_K(x') v(x') \delta(x - x') dx' = \rho_K(x) v(x) \quad N \to \infty \end{aligned} \tag{4.162}$$

Then equation (4.159) for $N \to \infty$ should be

$$\frac{1}{a^2}\frac{\partial^2 v}{\partial t^2} - \frac{\partial^2 v}{\partial x^2} = -\frac{1}{a^2\rho_0}\frac{\rho_M}{S}\frac{\partial^2 v}{\partial t^2} - \frac{\rho_K}{a^2\rho_0 S}v \tag{4.163}$$

Posing

$$\omega(x) = \sqrt{\frac{\rho_K(x)}{\rho_0 S}} \quad \text{and} \quad n(x) = \sqrt{1 + \frac{\rho_M(x)}{\rho_0 S}} \tag{4.164}$$

equation (4.163) become

$$n^2(x)\frac{\partial^2 v}{\partial t^2} - a^2\frac{\partial^2 v}{\partial x^2} + \omega^2(x)v = 0 \tag{4.165}$$

Consider the Cauchy problem

$$\begin{aligned} &\frac{1}{a^2}\frac{\partial^2 v}{\partial t^2} - \frac{\partial^2 v}{\partial x^2} = \frac{1}{a^2\rho_0}\sum_{j=1}^{N}\dot{\sigma}_j\,\delta_{s_j} \\ &v(x,0) = f(x) \\ &\left.\frac{\partial v}{\partial t}\right|_{t=0} = g(x) \end{aligned} \tag{4.166}$$

The solution of (4.166) is

$$\begin{aligned} v(x,t) = &\frac{1}{2}\left(f(x-at) + f(x+at)\right) + \frac{1}{2a}\int_{x-at}^{x+at} g(x')dx' + \\ &+ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x,t;x',t')\frac{1}{a^2\rho_0}\sum_{j=1}^{N}\dot{\sigma}_j(t')\,\delta(x'-s_j)dt'dx' \end{aligned} \tag{4.167}$$

where

$$G(x,t;x',t') = \frac{a}{2}\,\Theta\left(t - t' - \frac{|x-x'|}{a}\right), \tag{4.168}$$

and $\Theta(x)$ is the Heaviside function,

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} \tag{4.169}$$

It is easy to check that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x,t;x',t')\dot{\sigma}_j(t')\,\delta(x'-s_j)dt'dx' = \frac{a}{2}\,\sigma_j\left(t - \frac{|x-s_j|}{a}\right) \tag{4.170}$$

Then the solution of the Cauchy problem (4.166) is

$$\begin{aligned} v(x,t) = &\frac{1}{2}\left(f(x-at) + f(x+at)\right) + \frac{1}{2a}\int_{x-at}^{x+at} g(x')dx' + \\ &+ \frac{1}{2a\rho_0}\sum_{j=1}^{N}\sigma_j\left(t - \frac{|x-s_j|}{a}\right) \end{aligned} \tag{4.171}$$

From equation (4.149)

$$\sigma_j(t) = -\frac{K_j}{S} y_j(t) - \frac{M_j}{S} \dot{z}_j(t) \tag{4.172}$$

$$= -\frac{K_j}{S} u(s_j, t) - \frac{M_j}{S} \dot{v}(s_j, t) \tag{4.173}$$

where $u(x,t)$ satisfies $v = \frac{\partial u}{\partial t}$. Taking the limit $N \to \infty$

$$\begin{aligned} &\sum_{j=1}^{N} \sigma_j \left(t - \frac{|x - s_j|}{a} \right) \to \\ &\to -\rho_0 \int_{-\infty}^{\infty} \omega^2(x') u \left(x', t - \frac{|x - x'|}{a} \right) dx' + \\ &-\rho_0 \int_{-\infty}^{\infty} \gamma(x') \dot{v} \left(x', t - \frac{|x - x'|}{a} \right) dx' \quad N \to \infty \end{aligned} \tag{4.174}$$

with $\gamma(x) = \rho_M(x)/(\rho_0 S)$. It is possible to verify that

$$\begin{aligned} v(x,t) = &\frac{1}{2} \left(f(x - at) + f(x + at) \right) + \frac{1}{2a} \int_{x-at}^{x+at} g(x') dx' + \\ &- \frac{1}{2a} \int_{-\infty}^{\infty} \left[\omega^2(x') u \left(x', t - \frac{|x - x'|}{a} \right) + \gamma(x') \dot{v} \left(x', t - \frac{|x - x'|}{a} \right) \right] dx' \end{aligned} \tag{4.175}$$

is the solution of the limit Cauchy problem

$$\begin{aligned} &n^2(x) \frac{\partial^2 v}{\partial t^2} - a^2 \frac{\partial^2 v}{\partial x^2} + \omega^2(x) v = 0 \\ &v(x, 0) = f(x) \\ &\left. \frac{\partial v}{\partial t} \right|_{t=0} = g(x) \end{aligned} \tag{4.176}$$

notice that $n^2(x) = 1 + \gamma(x)$.

Conclusions

Some applications of point interactions to quantum and classical systems have been discussed in this thesis work. Although in very different frameworks the subjects under investigation were addressed to give quantitative estimates on the behavior of subsystems coupled with an environment by direct analysis of the dynamics of the whole system.

Because of the fact that they generate explicitly computable dynamics point interactions have revealed a powerful tool to reach our goal.

In the analysis of quantum systems the aim was to analyze the specific process with which interaction with the environment leads a subsystem initially in a pure state to evolve in a statistical mixture. This kind of problems is the core of the decoherence program.

In three dimensions, an approximate formula describing an event of scattering between two quantum particles in the limit of small mass ratio, the Joos and Zeh formula, has been proved. The control of the approximation is significantly stronger with point interactions than with generic smooth potential. In the model the light particle played the role of the environment. By using the approximated dynamics and tracing out the light particle's degrees of freedom an estimate of the suppression of the off-diagonal terms in the reduced density matrix has been obtained. Given a factorized initial state, with the light particle described by $\exp(|x|^2/(2\sigma^2))/(\pi\sigma^2)^{3/4}$ and the heavy particle in a coherent superposition of two wave packets centered in x_0 and $-x_0$ with momentum respectively p_0 and $-p_0$ heading toward the origin, it has been shown that the maximum effect of decoherence takes place on distances of the order of σ. The above mentioned results have been published in *Journal of physics A: mathematical and general*, [15].

A better model of environment should consist of N light particles. It is expected that the decoherence effects increase exponentially with N. For generic smooth potential this type of result was proved by R. Adami, R. Figari, D. Finco and A. Teta (preprint in preparation).

Moreover one and three dimensional models of interaction between a quantum particle and a localized spin have been proposed. The entire class of point interactions that can be obtained as singular perturbations of an assigned "free" dynamics has been characterized. The decoherence effects obtained by tracing out both the spin and the particle's degrees of freedom have been estimated. This has been done by choosing a particular subfamily of interacting Hamiltonians for which the generator of the dynamics was shown to be explicitly computable. The model proposed has revealed an interesting tool to investigate decoherence dynamically induced by the interaction. A paper containing these results is in preparation.

In principle it is possible to evaluate explicitly the suppression of off-diagonal terns in the reduced density matrix. As in the analysis of decoherence induced by scattering it is expected that an environment made up of N (even non interacting) spins will produce an exponential growth of the effects of decoherence. This result seems in reach without particular technical difficulties and it will be the subject of future work.
G. Sewell [45] suggested recently that an environment of N interacting spins would be more effective in inducing decoherence. It is conceivable that, as it happens to the supersaturated alcohol vapour of a cloud chamber, a system of spins in a metastable state would "decay" in a different way depending on the state of the particle. In this way an enhancement of the effects of decoherence would result. The idea of Sewell is very interesting even if the technical difficulties in controlling a system of N interacting spins seems overwhelming difficult.
In chapter 4 the results on a system of a finite and infinite number of mechanical oscillators in one dimension coupled with their own acoustic field have been presented. As it was mentioned in the introduction to the second part of this thesis, this is an acoustical version of the long standing open problem of the search of a complete theory of the electromagnetic field together with its point sources.
A completely new formulation of the problem in terms of point perturbations of a "free" operator on the Hilbert space of finite energy states has been proposed. In particular the problem of the transmission of acoustical waves across a periodical array of identical oscillators has been solved and the band structure completely characterized.
These results have been collected in the paper [16] submitted some months ago to the *Journal of Mathematical Physics*. The article is still under review.
The effective equation for the continuum limit of infinitely many mechanical oscillators has also been found.
In dimension three a model for a thin elastic shell with the fluid filling its inside and outside is available but no non-trivial limit of zero radius seems to exist. On the other hand the continuum limit should be non-trivial and will be analyzed in future work.
It is worth mentioning that there is a growing interest in the search of physical models of musical instruments.The most challenging goal of this program is the quantitative analysis of the mechanism of diffusion of energy on the infinitely many degrees of freedom of the oscillators and the acoustic field. Within this program what we have done may be considered a toy model.

Appendix A

Self-Adjoint Extensions of Symmetric Operators

In literature exist beautiful and comprehensive monographs on von Neumann's theory of deficiency indices and Krein's theory of self-adjoint extensions (see e.g. [5] and [40]), in this appendix we just state the main results.

A.1 Von Neumann formula

Let A_0 be a closed symmetric operator on a Hilbert space $\mathcal{H}$ and A_0^* its adjoint. Given $z \in \mathbb{C}\backslash\mathbb{R}$ we indicate with $\mathcal{K}^z(A_0)$ the eigenspace of A_0^* relative to the eigenvalue z

$$\mathcal{K}^z(A_0) = \mathrm{Ker}(A_0^* - zI)\,. \tag{A.1}$$

It is possible to show (see e.g. Theorem X.1 [40]) that the dimension of $\mathcal{K}^z$ is constant as z varies throughout the open upper half-plane or throughout the open lower half plane.

Conventionally $\mathcal{K}^i$ and $\mathcal{K}^{-i}$ play a special role and are referred to as *deficiency subspaces*. Numbers $n_+(A_0)$ and $n_-(A_0)$, defined as $n_+ = \dim[\mathcal{K}^i]$ and $n_- = \dim[\mathcal{K}^{-i}]$ are called *deficiency indices*, they are two non negative integers and it is possible to have n_+ and/or n_- equal infinity. To know the deficiency indices is equivalent to know the dimension of $\mathcal{K}^z$ for every $z \in \mathbb{C}\backslash\mathbb{R}$.

The knowledge of the deficiency indices gives precise indications about the self-adjointness of the operator and the realizability of self-adjoint extensions. This is due to the existence of a general decomposition formula for the domain of A_0^* often quoted as von Neumann formula, stating that if A_0 is a densely defined symmetric operator on a separable Hilbert space then for all $z \in \mathbb{C}\backslash\mathbb{R}$

$$D(A_0^*) = D(A_0) \oplus \mathcal{K}^z(A_0) \oplus \mathcal{K}^{\bar{z}}(A_0)\,. \tag{A.2}$$

Then it is not hard to convince ourselves that A_0 is self-adjoint if and only if $n_+(A_0) = n_-(A_0) = 0$, in fact, A_0 is symmetric and $D(A_0) = D(A_0^*)$.

If $n_+ = n_- > 0$ formula (A.2) suggests the strategy to find the self-adjoint extensions of A_0. In fact from (A.2) if $\psi \in D(A_0^*)$

$$\psi = \psi_0 + \phi^z + \phi^{\bar{z}} \qquad \psi_0 \in D(A_0),\ \phi^z \in \mathcal{K}^z,\ \phi^{\bar{z}} \in \mathcal{K}^{\bar{z}} \tag{A.3}$$

and

$$A_0^*\psi = A_0\psi_0 + z\phi^z + \bar{z}\phi^{\bar{z}}\,. \tag{A.4}$$

If A is an extension of A_0 the following chain of inclusions holds

$$A_0 \subseteq A \subseteq A^* \subseteq A_0^* \tag{A.5}$$

and $D(A^*)$ must be obtained by $D(A_0^*)$ restricting the subspace $\mathcal{K}^z \oplus \mathcal{K}^{\bar{z}}$.
Suppose that $(\phi^z + \phi^{\bar{z}}) \in D(A^*)$, by straightforward calculations one can check that

$$\left(\phi^z + \phi^{\bar{z}}, A^*(\phi^z + \phi^{\bar{z}})\right) - \left(A^*(\phi^z + \phi^{\bar{z}}), \phi^z + \phi^{\bar{z}}\right) = (z - \bar{z})\left(\|\phi^z\|^2 - \|\phi^{\bar{z}}\|^2\right) \tag{A.6}$$

then A^* is symmetric if and only if $\phi^{\bar{z}} = U\phi^z$ with U isometric application from $\mathcal{K}^z$ to $\mathcal{K}^{\bar{z}}$, being $\mathrm{Dim}(\mathcal{K}^z) = \mathrm{Dim}(\mathcal{K}^{\bar{z}})$ application U will be unitary. By evaluating the deficiency indices it is easy to verify that operator A^U

$$D(A^U) = \{\psi = \psi_0 + \phi^z + U\phi^z :\ \psi_0 \in D(A_0)\,,\ \phi^z \in \mathcal{K}^z(A_0)\} \tag{A.7}$$

$$A^U(\psi_0 + \phi^z + U\phi^z) = A_0\psi_0 + z\phi^z + \bar{z}U\phi^z \tag{A.8}$$

is self-adjoint.
Such construction does not work if $n_+ \neq n_-$, then self-adjoint extensions of a symmetric operator A_0 exist if and only if $n_+(A_0) = n_-(A_0) > 0$ and every self-adjoint extension of A_0 is an element of a family of self-adjoint operators parameterized by unitary applications U between $\mathcal{K}^z(A_0)$ and $\mathcal{K}^{\bar{z}}(A_0)$. Given U, the corresponding self-adjoint operator A^U is defined by (A.7) and (A.8).

A.2 Krein's formula for the resolvent

With von Neumann theory every self-adjoint extension is defined by formulas (A.7) and (A.8). Often such definition is rather cryptic and not too useful in applications. For this reason we conclude this appendix with the Krein's formula for the resolvent that allows a different and more readable characterization of self-adjoint extensions.
Assume that A_0 is a densely defined, closed symmetric operator in $\mathcal{H}$ with deficiency indices (N, N). If A^U and A^V are two self-adjoint extensions of A_0 then exists an operator $\ddot{A}_0$ such that $\ddot{A}_0 \subseteq A^U$, $\ddot{A}_0 \subseteq A^V$ and $\ddot{A}_0$ extends any operator B that fulfills $B \subseteq A^U$, $B \subseteq A^V$, $\ddot{A}_0$ is called the maximal common part of A^U and A^V. The deficiency indices of $\ddot{A}_0$ are (M, M) with $0 < M \leq N$.
A set $\{\phi_1^z, \ldots, \phi_M^z\}$ of independent solutions of

$$\ddot{A}_0^*\phi^z = z\phi^z \qquad \phi^z \in D(\ddot{A}_0^*),\ z \in \mathbb{C}\backslash\mathbb{R} \tag{A.9}$$

is a basis for $\mathcal{K}^z(\ddot{A}_0)$. The Krein's formula for the resolvent relates the resolvents of A^U and A^V by

$$(A^U - z)^{-1} - (A^V - z)^{-1} = \sum_{m,n=1}^{M} \Gamma(z)^{-1}_{mn}(\phi_n^{\bar{z}}, \cdot)\phi_m^z \qquad z \in \rho(A^U) \cap \rho(A^V) \tag{A.10}$$

where $\rho(A^U)$ and $\rho(A^V)$ indicate the resolvent set of A^U and A^V respectively, $\Gamma(z)^{-1}$ is a non singular matrix for $z \in \rho(A^U) \cap \rho(A^V)$ satisfying

$$\Gamma(z)^* = \Gamma(\bar{z}) \qquad z \in \rho(A^U) \cap \rho(A^V) \tag{A.11}$$

where * indicates the Hermitian conjugate. Functions $\Gamma(z)_{mn}$ and ϕ_m^z, m, $n = 1, \ldots, M$, may be chosen to be analytic for $z \in \rho(A^U) \cap \rho(A^V)$. In fact ϕ_m^z may be defined as

$$\phi_m^z = \phi_m^{z_0} + (z - z_0)(A^V - z)^{-1}\phi_m^{z_0} \qquad m = 1, \ldots, M\,,\ z \in \rho(A^V) \tag{A.12}$$

where $\phi_m^{z_0}$, $m = 1, \ldots, M$, $z_0 \in \mathbb{C}\backslash\mathbb{R}$, are linearly independent solutions of equation (A.9) with $z = z_0$ and matrix $\Gamma(z)$ as

$$\Gamma(z)_{mn} = \Gamma(z')_{mn} - (z - z')(\phi_n^{\bar{z}}, \phi_m^{z'}) \qquad \begin{array}{l} m, n = 1, \ldots, M \\ z, z' \in \rho(A^U) \cap \rho(A^V) \end{array} \tag{A.13}$$

where ϕ_m^z, $m = 1, \ldots, M$ are defined according to (A.12).
It is important to underline that the von Neumann and Krein's theory represent two independent approaches to the same problem, the first focuses its attention on the definition of the domain of self-adjoint extensions the second gives the resolvent of self-adjoint extensions of a given symmetric operator.

Appendix B

Proof of Theorem 2.1

Following the same line as in [23] and [3] we prove theorem 2.1 in three steps each one consisting in the proof of a lemma.

Lemma B.1. *If condition 1 is satisfied then there exists a constant* $C_1 > 0$ *such that, for any* $t > 0$ *one has*

$$\|\Psi(t) - \Psi_1(t)\| \leq C_1\varepsilon \tag{B.1}$$

where we defined

$$\begin{aligned}\Psi_1(t; R, r) \equiv \int_{\mathbb{R}^6} dx'\, dy'\, e^{-i\frac{t}{1+\varepsilon}H}\left(\frac{R+\varepsilon r}{1+\varepsilon} - x'\right)\varphi(x')\times \\ \times\, e^{-i\frac{t(1+\varepsilon)}{\varepsilon}H_\alpha}(r-R, y')\chi(y'+x')\end{aligned} \tag{B.2}$$

Proof. Notice that $\Psi(t)$ is the result of the evolution generated by the Hamiltonian $\mathbf{H}_\alpha$ of the initial state $\Psi(0; x, y) = \varphi\left(x - \frac{\varepsilon y}{1+\varepsilon}\right)\chi\left(x + \frac{y}{1+\varepsilon}\right)$. Making use of the unitarity of the evolution we obtain

$$\|\Psi(t) - \Psi_1(t)\|^2 = \|\Psi(0) - \Psi_1(0)\|^2 = \tag{B.3}$$

$$= \int_{\mathbb{R}^6} dx\, dy\, \left|\varphi\left(x - \frac{\varepsilon y}{1+\varepsilon}\right)\chi\left(x + \frac{y}{1+\varepsilon}\right) - \varphi(x)\chi(x+y)\right|^2 \tag{B.4}$$

We get then the following estimate

$$\|\Psi(0) - \Psi_1(0)\|^2 \leq \varepsilon^2 \int_{\mathbb{R}^6} dx\, dy\, |y|^2 \left|\nabla_x\left(\varphi(x)\chi(x+y)\right)\right|^2 \tag{B.5}$$

The r.h.s. of the last inequality is finite for $\varphi \in H^{1,1}(\mathbb{R}^3)$ and $\chi \in H^{1,1}(\mathbb{R}^3)$ and the proof is completed with

$$C_1^2 \equiv \int_{\mathbb{R}^6} dx\, dy\, |y|^2 \left|\nabla_x\left(\varphi(x)\chi(x+y)\right)\right|^2 \tag{B.6}$$

□

As we mentioned before the evolution of the system in the limit of small ε has two different time scales. In the second lemma we quantify this statement giving a rigorous estimate of how much the free evolution of the scattering state $[\Omega_+^{-1}\chi](y)$ approximates the exact evolution.

Lemma B.2. *If condition 1 is satisfied then there exists a constant $C_2 > 0$ such that for any $t > 0$ one has*

$$\|\Psi_2(t) - \Psi_1(t)\| \leq C_2 \left(\frac{\varepsilon}{t}\right)^{\frac{3}{4}} \tag{B.7}$$

where

$$\begin{aligned}\Psi_2(t; R, r) \equiv \int_{\mathbb{R}^3} dx'\, e^{-i\frac{t}{1+\varepsilon}H}\left(\frac{R+\varepsilon r}{1+\varepsilon} - x'\right)\varphi(x') \times \\ \times \int_{\mathbb{R}^3} dy'\, e^{-i\frac{1+\varepsilon}{\varepsilon}tH}(r - R - y')\left[\Omega_+^{-1}\chi(\cdot + x')\right](y')\end{aligned} \tag{B.8}$$

Proof. Following the notation of [3] we define $\chi_x(y) \equiv \chi(x+y)$. By direct computation we have

$$\begin{aligned}\|\Psi_2(t) - \Psi_1(t)\|^2 = \int_{\mathbb{R}^6} dx\, dy \Bigg| \int_{\mathbb{R}^6} dx'\, dy' e^{-i\frac{t}{1+\varepsilon}H}(x - x')\,\varphi(x') \times \\ \times \left[e^{-i\frac{1+\varepsilon}{\varepsilon}tH}(y - y')\left[\Omega_+^{-1}\chi_{x'}\right](y') - e^{-i\frac{1+\varepsilon}{\varepsilon}tH_\alpha}(y, y')\chi_{x'}(y')\right]\Bigg|^2\end{aligned} \tag{B.9}$$

Define the unitary operator

$$\Omega_\tau^+ = e^{i\tau H_\alpha} e^{-i\tau H} \tag{B.10}$$

and its inverse

$$(\Omega_\tau^+)^{-1} = e^{i\tau H} e^{-i\tau H_\alpha}\,. \tag{B.11}$$

Using the unitarity of the free propagator e^{-itH} we obtain

$$\begin{aligned}\|\Psi_2(t) - \Psi_1(t)\|^2 = \int_{\mathbb{R}^3} dx |\varphi(x)|^2 \times \\ \times \int_{\mathbb{R}^3} dy \left| \left[\Omega_+^{-1}\chi_x\right](y) - \left[\left(\Omega^+_{\frac{1+\varepsilon}{\varepsilon}t}\right)^{-1}\chi_x\right](y)\right|^2\end{aligned} \tag{B.12}$$

Due to the unitarity of the operators Ω_τ^+ and Ω_+ we have

$$\left\|\left(\Omega_+^{-1} - (\Omega_\tau^+)^{-1}\right)\chi\right\|_{L^2(\mathbb{R}^3)} = \left\|\left(\Omega_+ - \Omega_\tau^+\right)\Omega_+^{-1}\chi\right\|_{L^2(\mathbb{R}^3)} \tag{B.13}$$

In the following we will prove that for any $\eta \in L^2_2(\mathbb{R}^3)$

$$\left\|\left(\Omega_+ - \Omega_\tau^+\right)\eta\right\|_{L^2(\mathbb{R}^3)} \leq \frac{C'}{\tau^{\frac{3}{4}}} \quad \text{for } \tau \to \infty \tag{B.14}$$

In fact from (2.7) we have

$$\left[\Omega_+\eta\right](x) = [\mathcal{F}_+^{-1}\mathcal{F}\eta](x) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^6} dk\, dy\, \Phi_+(x,k) e^{-iky}\eta(y) \tag{B.15}$$

whereas from its definition

$$\left[\Omega_\tau^+\eta\right](y) = \int_{\mathbb{R}^6} dz\, dy' e^{i\tau H_\alpha}(y, z) e^{-i\tau H}(z - y')\eta(y') \tag{B.16}$$

By explicit computation we have

$$\left(\Omega_+ - \Omega_\tau^+\right)\eta = W_0\eta + W_\alpha\eta \tag{B.17}$$

with

$$[W_0\eta](|x|) = \frac{2i}{(2\pi)^2}\frac{1}{|x|}\int_0^\infty \frac{1-e^{-i\frac{|x|^2-|y|^2}{4\tau}}}{|x|^2-|y|^2}g(|y|)d|y| \tag{B.18}$$

and

$$\begin{aligned}[W_\alpha\eta](|x|) = \frac{8\pi i\alpha}{(2\pi)^2}\frac{1}{|x|}\int_0^\infty d|y|\frac{g(|y|)}{|y|}\int_0^\infty ds\, e^{-is|x|}\sin s|y| \times \\ \times\left(\frac{1}{4\pi\alpha+is} - e^{-i\frac{|x|^2-|y|^2}{4\tau}}\sqrt{-i\pi\tau}e^{z^2}erfc(z)\right)\end{aligned} \tag{B.19}$$

with $z = \sqrt{-i\tau}\left(4\pi\alpha + is + i\frac{|x|}{2\tau}\right)$ and $g(|x|) = |x|^2\int \eta(|x|, x_\theta, x_\varphi)d\Omega_x$.
We start with an estimate for W_0. From (B.18) we have

$$\|W_0\eta\|^2_{L^2(\mathbb{R}^3)} \le \frac{16}{(2\pi)^3}\int_0^\infty |g(|y|)|^2 K_\tau(|y|)d|y| \tag{B.20}$$

where

$$K_\tau(|y|) = \frac{1}{16\tau^{\frac{3}{2}}}\int_0^\infty \frac{1-\cos\left(\xi - \frac{|y|^2}{4\tau}\right)}{\left(\xi - \frac{|y|^2}{4\tau}\right)^2}\frac{1}{\sqrt{\xi}}d\xi \le \tag{B.21}$$

$$\le \frac{1}{16\tau^{\frac{3}{2}}}\left[2 + \sqrt{\frac{|y|^2}{4\tau}+1}\right] \tag{B.22}$$

We obtain then

$$\|W_0\eta\|^2_{L^2(\mathbb{R}^3)} \le D_0\left[\frac{1}{\tau^{\frac{3}{2}}}\int_0^\infty |g(|y|)|^2 d|y| + \frac{1}{\tau^2}\int_0^\infty |g(|y|)|^2|y|d|y|\right] \tag{B.23}$$

The estimate for the term $W_\alpha\eta$ in (B.19) will be given in few steps. We write $W_\alpha\eta$ as the sum of four terms

$$\begin{aligned}[W_\alpha\eta](|x|) =& \frac{8\pi i\alpha}{(2\pi)^2}\frac{1}{|x|}\int_0^\infty d|y|\frac{g(|y|)}{|y|}\int_0^\infty ds\, e^{-is|x|}\sin s|y| e^{i\frac{|y|^2}{4\tau}} \times \\ &\times\left[\frac{e^{-i\frac{|y|^2}{4\tau}}-1}{4\pi\alpha+is} + \frac{1-e^{-i\frac{|x|^2}{4\tau}}}{4\pi\alpha+is} + \right. \\ &+ e^{-i\frac{|x|^2}{4\tau}}\left(\frac{1}{4\pi\alpha+is} - \frac{1}{4\pi\alpha+is+i\frac{|x|}{2\tau}}\right) + \\ &\left. - e^{-i\frac{|x|^2}{4\tau}}\left(\sqrt{-i\pi\tau}e^{z^2}erfc(z) - \frac{1}{4\pi\alpha+is+i\frac{|x|}{2\tau}}\right)\right]\end{aligned} \tag{B.24}$$

We have then

$$\|W_\alpha\eta\|^2_{L^2(\mathbb{R}^3)} \le W_1 + W_2 + W_3 + W_4 \tag{B.25}$$

with

$$W_1 = D\int_0^\infty d|x| \left| \int_0^\infty ds\, \frac{e^{-is|x|}}{4\pi\alpha + is} \mathcal{S}\Bigg(\frac{g(|y|)}{|y|} \Big(1 - e^{i\frac{|y|^2}{4\tau}}\Big), |y| \Bigg)(s) \right|^2 \tag{B.26}$$

$$W_2 = 2D\int_0^\infty d|x| \left(1 - \cos\frac{|x|^2}{4\tau}\right) \times$$
$$\times \left| \int_0^\infty ds\, \frac{e^{-is|x|}}{4\pi\alpha + is} \mathcal{S}\left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right)(s) \right|^2 \tag{B.27}$$

$$W_3 = \frac{D}{4\tau^2}\int_0^\infty d|x|\, |x|^2 \times$$
$$\times \left| \int_0^\infty ds\, \frac{e^{-is|x|}}{(4\pi\alpha + is)(4\pi\alpha + is + i\frac{|x|}{2\tau})} \mathcal{S}\left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right)(s) \right|^2 \tag{B.28}$$

$$W_4 = D\int_0^\infty d|x| \left| \int_0^\infty ds\, e^{-is|x|} \left(\sqrt{-i\pi\tau} e^{z^2} erfc(z) - \frac{1}{4\pi\alpha + is + i\frac{|x|}{2\tau}} \right) \times \right.$$
$$\left. \times\, \mathcal{S}\left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right)(s) \right|^2 \tag{B.29}$$

where $D = \frac{16\alpha^2}{\pi}$ and $\mathcal{S}\big(f(|y|), |y|\big)(s) = \displaystyle\int_0^\infty \sin s|y| f(|y|) d|y|$ is the Fourier-sin-transform of $f(|y|)$. Let us define

$$h(s) = \begin{cases} \frac{1}{4\pi\alpha + is} \mathcal{S}\left(\frac{g(|y|)}{|y|} \left(1 - e^{i\frac{|y|^2}{4\tau}}\right), |y| \right)(s) & s \geq 0 \\ 0 & s < 0 \end{cases} \tag{B.30}$$

so that $W_1 = 2\pi D \|\hat{h}\|^2_{L^2((0,\infty))} \leq 2\pi D \|\hat{h}\|^2_{L^2(\mathbb{R})} = 2\pi D\, \|h\|^2_{L^2(\mathbb{R})}$, where $\hat{h}$ is the usual one dimensional Fourier transform of $h(s)$. A straightforward computation gives

$$W_1 \leq \frac{D_1}{\tau^2} \int_0^\infty |g(|y|)|^2\, |y|^2 d|y| \tag{B.31}$$

It is easily seen from the definition of W_2 that

$$W_2 = 2D\int_0^\infty d|x| \frac{1 - \cos\frac{|x|^2}{4\tau}}{(1 + |x|^2)^2} \times$$
$$\times \left| \int_0^\infty ds\, \frac{(1 - \frac{d^2}{ds^2}) e^{-is|x|}}{4\pi\alpha + is} \mathcal{S}\left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right)(s) \right|^2 \tag{B.32}$$

An integration by parts in the variable s and an estimate of the integral in the variable $|x|$ for large τ give

$$W_2 \leq \frac{D}{\tau^{\frac{3}{2}}} \Bigg\{ \frac{1}{(4\pi\alpha)^2} \int_0^\infty d|y| |g(|y|)|^2 +$$
$$+ \int_0^\infty ds \left| \left(1 - \frac{d^2}{ds^2}\right) \frac{\mathcal{S}\left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right)(s)}{(4\pi\alpha + is)} \right|^2 \Bigg\} \tag{B.33}$$

We rewrite W_3 in the following way

$$W_3 = \frac{D}{4\tau^2}\int_0^\infty d|x| \left|\frac{|x|}{1+|x|^2}\right|^2 \times$$
$$\times \left|\int_0^\infty ds\, \frac{(1-\frac{d^2}{ds^2})e^{-is|x|}}{(4\pi\alpha+is)(4\pi\alpha+is+i\frac{|x|}{2\tau})}\mathcal{S}\left(\frac{g(|y|)}{|y|}e^{i\frac{|y|^2}{4\tau}},|y|\right)(s)\right|^2 \quad \text{(B.34)}$$

and we use the inequality $\left|\frac{d^m}{ds^m}\frac{1}{4\pi\alpha+is+i\frac{|x|}{2\tau}}\right|^2 \leq \left|\frac{d^m}{ds^m}\frac{1}{4\pi\alpha+is}\right|^2 \quad \forall\tau\geq 0,\ \forall m\in\mathbb{N}_0$ and $\forall x\in\mathbb{R}^3$, to obtain

$$W_3 \leq \frac{D}{\tau^2}\left\{\frac{1}{(4\pi\alpha)^4}\int_0^\infty d|y||g(|y|)|^2 + \right.$$
$$\left. + \int_0^\infty ds\left|\left(1-\frac{d^2}{ds^2}\right)\frac{\mathcal{S}\left(\frac{g(|y|)}{|y|}e^{i\frac{|y|^2}{4\tau}},|y|\right)(s)}{(4\pi\alpha+is)^2}\right|^2\right\} \quad \text{(B.35)}$$

In the W_4 term for $\tau\to\infty$ we have $|z|\to\infty$ and we can use the asymptotic expansion $e^{z^2}erfc(z)-\frac{1}{\sqrt{\pi}z} = -\frac{1}{2\sqrt{\pi}z^3}+o\left(\frac{1}{z^5}\right)$. From the inequality

$$\left|\frac{d^m}{dz^m}\left(e^{z^2}erfc(z)-\frac{1}{\sqrt{\pi}z}\right)\right| \leq \left|\frac{1}{\sqrt{\pi}z^{3+m}}\right| \quad \text{for } |z|\to\infty \quad \text{(B.36)}$$

$\forall m\in\mathbb{N}_0$, we obtain

$$W_4 \leq \frac{D}{\tau^2}\int_0^\infty d|x|\frac{1}{1+|x|^2}\times$$
$$\times\int_0^\infty ds\left|\left(1-\frac{d}{ds}\right)\frac{1}{\left(4\pi\alpha+is+i\frac{|x|}{2\tau}\right)^3}\mathcal{S}\left(\frac{g(|y|)}{|y|}e^{i\frac{|y|^2}{4\tau}},|y|\right)(s)\right|^2 \quad \text{(B.37)}$$

With the same estimate used in (B.34) it is easily seen that

$$W_4 \leq \frac{\pi D}{2\tau^2}\int_0^\infty ds\left|\left(1-\frac{d}{ds}\right)\frac{1}{(4\pi\alpha+is)^3}\mathcal{S}\left(\frac{g(|y|)}{|y|}e^{i\frac{|y|^2}{4\tau}},|y|\right)(s)\right|^2 \quad \text{(B.38)}$$

Notice that if $\eta\in L_2^2(\mathbb{R}^3)$ all the integrals in the $(B.23)$, $(B.31)$, $(B.33)$, $(B.35)$, $(B.38)$ are finite and we get estimate (B.14).
From (B.12) and (B.13) in order to conclude the proof of lemma 2.2 we need to show that if the initial state satisfies condition A then $\eta=\Omega_+^{-1}\chi_x\in L_2^2(\mathbb{R}^3)$ for every $x\in\mathbb{R}^3$ and

$$\left\|\Omega_+^{-1}\chi_x\right\|_{L_2^2(\mathbb{R}^3)} \leq C'(1+|x|^2)^{\frac{1}{2}} \quad \text{(B.39)}$$

We omit the details of this last result that follows easily from an integration by parts in the explicit definition of the L_2^2 norm of $\Omega_+^{-1}\chi_x$. □

To conclude the proof of theorem 2.1 we will show that the evolution of the initial state $\varphi(x)[\Omega_+^{-1}\chi_x](y)$ according to the dynamics generated by the Hamiltonian

$\mathbf{H}$ approximate at the order ε the dynamics of the initial state $\varphi(R)[(\Omega_+^R)^{-1}\chi](r)$ generated by the Hamiltonian $\mathbf{H}^a$.
Using the identity

$$\begin{aligned}&e^{-i\frac{t}{1+\varepsilon}H}\left(\frac{\varepsilon(r-r')+(R-R')}{1+\varepsilon}\right)e^{-i\frac{1+\varepsilon}{\varepsilon}tH}(r-r'-(R-R'))=\\&=e^{-itH}(R-R')e^{-i\frac{t}{\varepsilon}H}(r-r')\end{aligned}\tag{B.40}$$

we obtain

$$\begin{aligned}\Psi_2(t;r,R)=&\int_{\mathbb{R}^6}dr'\,dR'\,e^{-itH}(R-R')e^{-i\frac{t}{\varepsilon}H}(r-r')\times\\&\times\varphi\left(\frac{\varepsilon r'+R'}{1+\varepsilon}\right)\left[\Omega_+^{-1}\chi\left(\frac{\varepsilon r'+R'}{1+\varepsilon}+\cdot\right)\right](r'-R')\end{aligned}\tag{B.41}$$

We prove the last lemma

Lemma B.3. *There exists a constant $C_3>0$ such that for any $t>0$ one has*

$$\|\Psi_2(t)-\Psi^a(t)\|\le C_3\varepsilon \tag{B.42}$$

Proof. Given the unitarity of the free propagator

$$\begin{aligned}\|\Psi_2(t)-\Psi^a(t)\|^2=&\int_{\mathbb{R}^6}dR\,dr\left|\varphi\left(\frac{\varepsilon r+R}{1+\varepsilon}\right)\left[\Omega_+^{-1}\chi\left(\frac{\varepsilon r+R}{1+\varepsilon}+\cdot\right)\right](r-R)+\right.\\&\left.-\varphi(R)\left[\Omega_+^{-1}\chi(R+\cdot)\right](r-R)\right|^2\end{aligned}\tag{B.43}$$

where we used the relation $\left[(\Omega_+^R)^{-1}\chi\right](r)=\left[\Omega_+^{-1}\chi_R\right](r-R)$. In the system of coordinates of the center of mass this reads

$$\begin{aligned}\|\Psi_2(t)-\Psi^a(t)\|^2=&\int_{\mathbb{R}^6}dx\,dy\left|\varphi(x)\left[\Omega_+^{-1}\chi(x+\cdot)\right](y)+\right.\\&\left.-\varphi\left(x-\frac{\varepsilon}{1+\varepsilon}y\right)\left[\Omega_+^{-1}\chi\left(x-\frac{\varepsilon}{1+\varepsilon}y+\cdot\right)\right](y)\right|^2\end{aligned}\tag{B.44}$$

In the limit of small ε we can write

$$\begin{aligned}\|\Psi_2(t)-\Psi^a(t)\|^2&\le\varepsilon^2\int_{\mathbb{R}^6}dx\,dy\,|y|^2\left|\nabla_x\left[\varphi(x)\Omega_+^{-1}\chi_x(y)\right]\right|^2\\&\le\varepsilon^2\left((\diamond\mathbf{1})+(\diamond\mathbf{2})\right)\end{aligned}\tag{B.45}$$

Let us prove that the terms $(\diamond\mathbf{1})$, $(\diamond\mathbf{2})$ in (B.45) are finite. Using the definition (2.7) of Ω_+^{-1} and the explicit form of the generalized functions $\Phi_+(x,k)$ we obtain

$$\begin{aligned}(\diamond\mathbf{1})=&\int_{\mathbb{R}^6}dx\,dy\,\left|\nabla_x\varphi(x)\right|^2|y|^2\left|\Omega_+^{-1}\chi_x(y)\right|^2=\\=&\left(\frac{1}{2\pi}\right)^3\int_{\mathbb{R}^6}dx\,dk\,\left|\nabla_x\varphi(x)\right|^2\times\\&\times\left|\nabla_k\int_{\mathbb{R}^3}dz\,\left(e^{-ikz}+\frac{1}{4\pi\alpha-i|k|}\frac{e^{i|k||z|}}{|z|}\right)\chi_x(z)\right|^2\le(\diamond\mathbf{3})+(\diamond\mathbf{4})\end{aligned}\tag{B.46}$$

The estimate of the term ($\diamond\mathbf{3}$) follows easily

$$
\begin{aligned}
(\diamond\mathbf{3}) = &\left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx\, |\nabla_x \varphi(x)|^2 \int_{\mathbb{R}^3} dz\, \big| |z| \chi_x(z) \big|^2 \leq \\
\leq &\left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx\, |\nabla_x \varphi(x)|^2 \int_{\mathbb{R}^3} dz\, \big| |z| \chi_x(z) \big| + \\
&+ \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx\, |\nabla_x \varphi(x)|^2\, |x|^2\, \|\chi(z)\|^2_{L^2(\mathbb{R}^3)}
\end{aligned}
\tag{B.47}
$$

For the term ($\diamond\mathbf{4}$) we have

$$
\begin{aligned}
(\diamond\mathbf{4}) = &\left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^6} dx\, dk\, |\nabla_x \varphi(x)|^2 \left| \frac{d}{d|k|} \int_{\mathbb{R}^3} dz\, \frac{1}{4\pi\alpha - i|k|} \frac{e^{i|k||z|}}{|z|} \chi_x(z) \right|^2 \leq \\
\leq &(\diamond\mathbf{5}) + (\diamond\mathbf{6})
\end{aligned}
\tag{B.48}
$$

with

$$
(\diamond\mathbf{5}) = \int_{\mathbb{R}^6} dx\, dk\, \frac{|\nabla_x \varphi(x)|^2}{((4\pi\alpha)^2 + |k|^2)^2} \left| \int_{\mathbb{R}^3} dz\, \frac{e^{i|k||z|}}{|z|} \chi_x(z) \right|^2
\tag{B.49}
$$

In (B.49) the only problem is represented by the integral in the variable z. Making explicit the x dependence of $\chi_x(z)$ we have

$$
\begin{aligned}
&\left| \int_{\mathbb{R}^3} dz\, \frac{e^{i|k||z|}}{|z|} \chi(z+x) \right|^2 = \left| \int_{\mathbb{R}^3} d\xi\, \frac{e^{i|k||\xi - x|}}{|\xi - x|(1+|\xi|^2)^{\frac{1}{2}}} \chi(\xi)(1+|\xi|^2)^{\frac{1}{2}} \right|^2 \leq \\
&\leq \left(\int_{\mathbb{R}^3} d\xi\, |\chi(\xi)|^2 (1+|\xi|^2) \right) \left(\int_{\mathbb{R}^3} d\xi\, \frac{1}{|\xi - x|^2 (1+|\xi|^2)} \right) = \\
&= \|(1+|\cdot|^2)^{\frac{1}{2}} \chi\|^2_{L^2(\mathbb{R}^3)} \left\| \frac{1}{|\cdot|(1+|\cdot + x|^2)^{\frac{1}{2}}} \right\|^2_{L^2(\mathbb{R}^3)}
\end{aligned}
\tag{B.50}
$$

where we used Holder's inequality. An explicit computation shows that

$$
\left\| \frac{1}{|\cdot|(1+|\cdot + x|^2)^{\frac{1}{2}}} \right\|^2_{L^2(\mathbb{R}^3)} \leq \frac{\pi^2}{|x|}
\tag{B.51}
$$

We finally estimate the term

$$
(\diamond\mathbf{6}) = \int_{\mathbb{R}^6} dx\, dk\, \frac{|\nabla_x \varphi(x)|^2}{(4\pi\alpha)^2 + |k|^2} \left| \int_{\mathbb{R}^3} dz\, \chi_x(z) e^{-i|k||z|} \right|^2
\tag{B.52}
$$

To ensure convergence we need that the integral in the variable z goes to zero at infinity faster than $1/|k|^{1/2}$. In fact integrating by parts

$$
\begin{aligned}
&\left| \int_{\mathbb{R}^3} dz\, \chi(z+x) e^{i|k||z|} \right|^2 = \left| \int_{\mathbb{R}^3} d\xi\, \chi(\xi) \frac{-i}{|k|} \frac{\xi - x}{|\xi - x|} \nabla_\xi e^{i|k||\xi - x|} \right|^2 \leq \\
\leq &\frac{1}{|k|^2} \int_{\mathbb{R}^3} d\xi\, |\nabla_\xi \chi(\xi)|^2 + \frac{4}{|k|^2} \left| \int_{\mathbb{R}^3} d\xi\, \frac{e^{i|k||\xi - x|}}{|\xi - x|} \chi(\xi) \right|^2
\end{aligned}
\tag{B.53}
$$

We are left to show that also the term $(\diamond\mathbf{2})$

$$(\diamond\mathbf{2}) = \int_{\mathbb{R}^6} dx\, dy\, |\varphi(x)|^2 \, |y|^2 \left|\nabla_x \Omega_+^{-1} \chi_x(y)\right|^2 \tag{B.54}$$

is finite. Notice that

$$\left|\nabla_x \Omega_+^{-1} \chi_x(y)\right|^2 = \sum_{i=1}^{3} \left|\partial_{x_i} (\Omega_+^{-1} \chi_x)(y)\right|^2 = \sum_{i=1}^{3} \left|\Omega_+^{-1} f_{i,x}(y)\right|^2 \tag{B.55}$$

with $f_{i,x}(z) = \partial_{x_i} \chi_x(z) = \partial_{x_i} \chi(z+x) = f_i(z+x)$. It follows that the estimate for $(\diamond\mathbf{2})$ can be obtained with the same procedure used for $(\diamond\mathbf{1})$, the only difference being that we must replace $\chi(x+z)$ with $\nabla\chi(x+z)$. We conclude that all the integrals are finite if condition 1 is satisfied. $\square$

Appendix C

Characterization of Self-Adjoint Extensions of H_0

In this appendix we characterize all the self-adjoint perturbations of the operator (3.5) in one and three dimensions. The structure of the family of Hamiltonians obtained as point perturbations of the "free" Hamiltonian introduced in (3.5) is derived by using the theory of self-adjoint extensions described in appendix A.

C.1 The deficiency subspaces

Consider the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^2 \tag{C.1}$$

an element of $\mathcal{H}$ can be always written as

$$\Psi = \sum_{\sigma=\pm} \psi_\sigma(x) \otimes \chi_\sigma \tag{C.2}$$

where $\psi_\sigma(x) \in L^2(\mathbb{R}^d)$ while $\chi_\pm$ are the normalized vectors in $\mathbb{C}^2$ satisfying $\sigma_x \chi_\pm = \pm\chi_\pm$. Where σ_x is the Pauli matrix that in the standard basis of the spin operator $\vec{\sigma}$ is expressed by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{C.3}$$

The scalar product in $\mathcal{H}$ is

$$\langle \Psi_1, \Psi_2 \rangle = \sum_{\sigma=\pm} (\psi_{1\sigma}, \psi_{2\sigma}), \tag{C.4}$$

where $(\,\cdot\,,\cdot\,)$ indicates the standard product in $L^2(\mathbb{R}^d)$.
On $\mathcal{H}$ consider the symmetric operator

$$D(H_0) = C_0^\infty(\mathbb{R}^d) \otimes \mathbb{C}^2 \qquad H_0 = -\Delta \otimes \mathbb{I} + \mathbb{I} \otimes \alpha\,\sigma_x \qquad \alpha \in \mathbb{R}\,. \tag{C.5}$$

A set of independent solutions of equation

$$(H_0^* - z)\Phi^z = 0 \qquad z \in \mathbb{C}\backslash\mathbb{R},\ \Phi^z \in \mathcal{H} \tag{C.6}$$

is

$$\begin{cases} \Phi^z_{\pm} = G^{z\mp\alpha}(x-y) \otimes \chi_{\pm} \\ \Phi^z_{1\pm} = (G^{z\mp\alpha})'(x-y) \otimes \chi_{\pm} \end{cases} \qquad z \in \mathbb{C}\backslash\mathbb{R} \qquad d=1 \tag{C.7}$$

$$\Phi^z_{\pm} = G^{z\mp\alpha}(x-y) \otimes \chi_{\pm} \qquad z \in \mathbb{C}\backslash\mathbb{R} \qquad d=3 \tag{C.8}$$

Function $G^z(x)$ is the integral kernel of the resolvent of the free Laplacian in d dimensions, i.e. the inverse Fourier transform of

$$\frac{1}{k^2 - z} \qquad z \in \mathbb{C}\backslash\mathbb{R} \tag{C.9}$$

in dimension d, its explicit expression is

$$G^z(x) = \begin{cases} i\dfrac{e^{i\sqrt{z}|x|}}{2\sqrt{z}} & d=1 \\ \\ \dfrac{e^{i\sqrt{z}|x|}}{4\pi|x|} & d=3 \end{cases} \qquad z \in \mathbb{C}\backslash\mathbb{R}^+ \qquad \mathrm{Im}\,(\sqrt{z}) > 0 \tag{C.10}$$

$(G^z)'$ indicates the first derivative of G^z with respect to x

$$(G^z)'(x) = -\mathrm{sgn}(x)\frac{e^{i\sqrt{z}|x|}}{2} \qquad z \in \mathbb{C}\backslash\mathbb{R}^+ \qquad \mathrm{Im}\,(\sqrt{z}) > 0 \qquad d=1 \tag{C.11}$$

From (C.7) and (C.8) one easily obtains the deficiency indices n_+ and n_-. For $d=1$, $n_+ = n_- = 4$ while for $d=3$, $n_+ = n_- = 2$.
Then from the general theory of self-adjoint extensions one obtains that both in one and three dimensions exist non trivial self-adjoint extensions of H_0. For $d = 1$ the situation is very rich and the family of self-adjoint extensions is parameterized by 16 real parameters, while for $d = 3$ one obtains a 4-real parameters family of self-adjoint extensions of H_0.
For $d = 1$ we indicate with $\{e_+, e_-, e_{1+}, e_{1-}\}$ the orthonormal basis of the deficiency space $\mathcal{K}^i$

$$e_{\pm} = \frac{G^{i\mp\alpha}(x-y)}{\|G^{i\mp\alpha}\|} \otimes \chi_{\pm} \tag{C.12}$$

$$e_{1\pm} = \frac{(G^{i\mp\alpha})'(x-y)}{\|(G^{i\mp\alpha})'\|} \otimes \chi_{\pm} \tag{C.13}$$

and with $\{\tilde{e}_+, \tilde{e}_-, \tilde{e}_{1+}, \tilde{e}_{1-}\}$ the orthonormal basis of the deficiency space $\mathcal{K}^{-i}$

$$\tilde{e}_{\pm} = -\frac{G^{-i\mp\alpha}(x-y)}{\|G^{-i\mp\alpha}\|} \otimes \chi_{\pm} \tag{C.14}$$

$$\tilde{e}_{1\pm} = -\frac{(G^{-i\mp\alpha})'(x-y)}{\|(G^{-i\mp\alpha})'\|} \otimes \chi_{\pm} \tag{C.15}$$

For $d = 1$

$$\frac{G^z(x)}{\|G^z\|} = i\frac{\sqrt{|z|\text{Im}\,(\sqrt{z})}}{\sqrt{z}}e^{i\sqrt{z}|x|} \qquad \text{Im}\,(\sqrt{z}) > 0 \tag{C.16}$$

$$\frac{(G^z)'(x)}{\|(G^z)'\|} = -\sqrt{\text{Im}\,(\sqrt{z})}\text{sgn}(x)\frac{e^{i\sqrt{z}|x|}}{2} \qquad \text{Im}\,(\sqrt{z}) > 0 \tag{C.17}$$

Notice that

$$\|G^z\| = \|G^{\bar{z}}\| \qquad \|(G^z)'\| = \|(G^{\bar{z}})'\| \tag{C.18}$$

For $d = 3$ we indicate with $\{f_+, f_-\}$ the orthonormal basis of the deficiency space $\mathcal{K}^i$

$$f_\pm = \frac{G^{i\mp\alpha}(x-y)}{\|G^{i\mp\alpha}\|} \otimes \chi_\pm \tag{C.19}$$

and with $\left\{\tilde{f}_+, \tilde{f}_-\right\}$ the orthonormal basis of the deficiency space $\mathcal{K}^{-i}$

$$\tilde{f}_\pm = -\frac{G^{-i\mp\alpha}(x-y)}{\|G^{-i\mp\alpha}\|} \otimes \chi_\pm \tag{C.20}$$

for $d = 3$

$$\frac{G^z(x)}{\|G^z\|} = \sqrt{\frac{\text{Im}\,(\sqrt{z})}{2\pi}}\frac{e^{i\sqrt{z}|x-y|}}{|x-y|} \qquad \text{Im}\,(\sqrt{z}) > 0 \tag{C.21}$$

and $\|G^z\| = \|G^{\bar{z}}\|$

Following formulas (A.7) and (A.8) one obtains that the family of self-adjoint extensions of H_0 is parameterized by the unitary applications U from $\mathcal{K}^i$ to $\mathcal{K}^{-i}$. We indicate the generic element of this family with H^U and

$$\begin{gathered} D(H^U) = \left\{\Psi \in \mathcal{H} :\ \Psi = \Psi_0 + \Phi^i + U\Phi^i;\ \Psi_0 \in D(H_0),\ \Phi^i \in \mathcal{K}^i\right\} \\ H^U\Psi = H_0\Psi_0 + i\Phi^i - iU\Phi^i \end{gathered} \tag{C.22}$$

C.2 One dimension

For $d = 1$ a generic vector in $\mathcal{K}^i$ can be written as

$$\Phi^i = a_1 e_+ + a_2 e_- + a_3 e_{1+} + a_4 e_{1-} \tag{C.23}$$

where $a_j \in \mathbb{C}$ and the corresponding vector in K^{-i} by U is

$$U\Phi^i = \tilde{a}_1\tilde{e}_+ + \tilde{a}_2\tilde{e}_- + \tilde{a}_3\tilde{e}_{1+} + \tilde{a}_4\tilde{e}_{1-} \tag{C.24}$$

with $\tilde{a}_j = \sum_k U_{jk}a_k$, where U_{jk} is the four dimensional unitary matrix representing the application U in the basis $\{e_+, e_-, e_{1+}, e_{1-}\}$ and $\{\tilde{e}_+, \tilde{e}_-, \tilde{e}_{1+}, \tilde{e}_{1-}\}$. We want to characterize different self-adjoint extensions in terms of the boundary conditions satisfied by the particle wave function in the corresponding domains. The more general 4×4 unitary matrix has 16 real independent parameters, we choose a particular form of the unitary matrix with only 8 independents real parameters. Consider the matrix U

$$U = \begin{pmatrix} U_2 & O_2 \\ O_2 & V_2 \end{pmatrix} \quad U_2 = \begin{pmatrix} e^{i\theta}\cos\omega & e^{i(\theta+\rho)}\sin\omega \\ -e^{i(\varphi-\rho)}\sin\omega & e^{i\varphi}\cos\omega \end{pmatrix}$$
$$V_2 = \begin{pmatrix} e^{i\theta_1}\cos\omega_1 & e^{i(\theta_1+\rho_1)}\sin\omega_1 \\ -e^{i(\varphi_1-\rho_1)}\sin\omega_1 & e^{i\varphi_1}\cos\omega_1 \end{pmatrix} \tag{C.25}$$

where θ, ρ, φ, ω, θ_1, ρ_1, φ_1, ω_1 are real parameters. While O_2 is the 2×2 matrix with all zero entries.
We write the generic element in the domain of H^U as

$$\Psi = \psi_+(x) \otimes \chi_+ + \psi_-(x) \otimes \chi_- \tag{C.26}$$

In general functions $\psi_+(x)$ and $\psi_-(x)$ are not continuous and they do not have continuous derivative in $x = y$. With straightforward calculations one can check that the boundary conditions satisfied by the right and left limits of the functions ψ_+, ψ_- and of their derivatives are

$$\begin{aligned}
&\frac{d\psi_+}{dx}(y^+) - \frac{d\psi_+}{dx}(y^-) = c_1\left(\psi_+(y^+) + \psi_+(y^-)\right) + c_2\left(\psi_-(y^+) + \psi_-(y^-)\right) \\
&\frac{d\psi_-}{dx}(y^+) - \frac{d\psi_-}{dx}(y^-) = c_3\left(\psi_+(y^+) + \psi_+(y^-)\right) + c_4\left(\psi_-(y^+) + \psi_-(y^-)\right) \\
&\psi_+(y^+) - \psi_+(y^-) = d_1\left(\frac{d\psi_+}{dx}(y^+) + \frac{d\psi_+}{dx}(y^-)\right) + d_2\left(\frac{d\psi_-}{dx}(y^+) + \frac{d\psi_-}{dx}(y^-)\right) \\
&\psi_-(y^+) - \psi_-(y^-) = d_3\left(\frac{d\psi_+}{dx}(y^+) + \frac{d\psi_+}{dx}(y^-)\right) + d_4\left(\frac{d\psi_-}{dx}(y^+) + \frac{d\psi_-}{dx}(y^-)\right)
\end{aligned} \tag{C.27}$$

with

$$\begin{aligned}
c_1 &= \frac{(1 - e^{i\theta}\cos\omega)(e^{i\varphi}\cos\omega\sqrt{\alpha+i} - \sqrt{\alpha-i}) - e^{i(\theta+\varphi)}\sin^2\omega\sqrt{\alpha+i}}{C} \\
c_2 &= \sqrt{\frac{\mathrm{Im}\,(\sqrt{i-\alpha})}{\mathrm{Im}\,(\sqrt{i+\alpha})}}\,\frac{-ie^{i(\theta+\rho)}\sin\omega(\sqrt{\alpha+i} + (\sqrt{\alpha-i})}{C} \\
c_3 &= \sqrt{\frac{\mathrm{Im}\,(\sqrt{i+\alpha})}{\mathrm{Im}\,(\sqrt{i-\alpha})}}\,\frac{e^{i(\varphi-\rho)}\sin\omega(\sqrt{\alpha-i} - \sqrt{\alpha+i})}{C} \\
c_4 &= i\frac{(1 - e^{i\varphi}\cos\omega)(e^{i\theta}\cos\omega\sqrt{\alpha-i} + \sqrt{\alpha+i}) - e^{i(\theta+\varphi)}\sin^2\omega\sqrt{\alpha-i}}{C} \\
d_1 &= \frac{(1 - e^{i\theta_1}\cos\omega_1)(e^{i\varphi_1}\cos\omega_1\sqrt{\alpha-i} - \sqrt{\alpha+i}) - e^{i(\theta_1+\varphi_1)}\sin^2\omega_1\sqrt{\alpha-i}}{D} \\
d_2 &= \sqrt{\frac{\mathrm{Im}\,(\sqrt{i-\alpha})}{\mathrm{Im}\,(\sqrt{i+\alpha})}}\,\frac{-ie^{i(\theta_1+\rho_1)}\sin\omega_1(\sqrt{\alpha+i} + (\sqrt{\alpha-i})}{D} \\
d_3 &= \sqrt{\frac{\mathrm{Im}\,(\sqrt{i+\alpha})}{\mathrm{Im}\,(\sqrt{i-\alpha})}}\,\frac{e^{i(\varphi_1-\rho_1)}\sin\omega_1(\sqrt{\alpha-i} - \sqrt{\alpha+i})}{D} \\
d_4 &= i\frac{(1 - e^{i\varphi_1}\cos\omega_1)(e^{i\theta_1}\cos\omega_1\sqrt{\alpha+i} + \sqrt{\alpha-i}) - e^{i(\theta_1+\varphi_1)}\sin^2\omega_1\sqrt{\alpha+i}}{C}
\end{aligned} \tag{C.28}$$

and

$$\begin{aligned}C =& \left(e^{i\theta}\cos\omega\frac{\sqrt{\alpha-i}}{\sqrt{1+\alpha^2}}+\frac{\sqrt{\alpha+i}}{\sqrt{1+\alpha^2}}\right)\left(e^{i\varphi}\cos\omega\frac{\sqrt{\alpha+i}}{\sqrt{1+\alpha^2}}-\frac{\sqrt{\alpha-i}}{\sqrt{1+\alpha^2}}\right)+\\ &-e^{i(\theta+\varphi)}\sin^2\omega\\ D =&(e^{i\theta_1}\cos\omega_1\sqrt{\alpha+i}+\sqrt{\alpha-i})(e^{i\varphi_1}\cos\omega_1\sqrt{\alpha-i}-\sqrt{\alpha+i})+\\ &-e^{i(\theta_1+\varphi_1)}\sin^2\omega_1\sqrt{1+\alpha^2}\end{aligned} \tag{C.29}$$

For both $\psi_+(x)$ and $\psi_-(x)$ the difference of the right and left limits in y of the derivatives depends only on the sum of the value of the right and left limits in y of the functions. In the same way the difference of the right and left limits of the functions $\psi_\pm(x)$ in y depends only on the sum of the right and left limits of the derivative in the same point. This happens because we chose the unitary matrix as a diagonal block matrix in which the diagonal elements are 2×2 unitary matrices.
The discontinuities of the functions $\psi_\pm(x)$ in y depend only on the parameters characterizing the 2×2 matrix V_2 while the discontinuities of the derivatives depend only on the parameters appearing in the 2×2 matrix U_2. This means that matrix U_2 is connected with δ-like perturbations (continuous functions with discontinuous derivative) while matrix V_2 is connected with δ'-like perturbations (discontinuous functions but with the same right and left limits of the derivatives in y). Constants c_1, c_4 do not depend on ρ as constants d_1, d_4 do not depend on ρ_1 then the parameters ρ and ρ_1 influence only the dependence of $\psi_+(x)$ on $\psi_-(x)$ and vice versa, because ρ and ρ_1 appear only in off-diagonal terms. Notice that there is a dependence of $\psi_+(x)$ on $\psi_-(x)$ and vice versa only if there are off diagonal terms.
In the following we discuss in detail some very special extensions.

C.2.1 Free dynamics

From (C.28) it is easy to check that if $U_{jk}=\delta_{jk}$ ($\omega=\theta=\varphi=\rho=\omega_1=\theta_1=\varphi_1=\rho_1=0$), functions $\psi_\pm(x)$ are continuous in y with their first derivative. Indicating with H the corresponding self-adjoint operator one has

$$D(H)=H^2(\mathbb{R})\otimes\mathbb{C}^2 \qquad H=-\Delta\otimes\mathbb{I}+\mathbb{I}\otimes\alpha\,\sigma_x \qquad \alpha\in\mathbb{R}\,. \tag{C.30}$$

H is the generator of the "free" dynamics.

C.2.2 δ-like interactions

A different way to characterize the singular perturbations of a given self-adjoint operator is to use the Krein's formula for the resolvent. In this section we show how to obtain the resolvent of a special class of self-adjoint singular perturbations of H, the one corresponding to vectors with wave function continuous but with discontinuous first derivative in y.
We indicate with H^Θ a generic self-adjoint perturbation of H in this class. From formula (A.10) we obtain that the resolvent of H^Θ can be written as

$$(H^\Theta-z)^{-1}=(H-z)^{-1}+\sum_{\sigma_1,\sigma_2=\pm}(\Gamma^\Theta(z))^{-1}_{\sigma_1\sigma_2}\langle\Phi^{\bar z}_{\sigma_2},\cdot\rangle\Phi^z_{\sigma_1} \qquad z\in\rho(H)\cap\rho(H^\Theta) \tag{C.31}$$

Where $\Phi^z_\pm$ are defined in (C.7) and $\Gamma^\Theta(z)$ is a matrix defined by

$$\Gamma^\Theta(z)_{\sigma_1\sigma_2} - \Gamma^\Theta(w)_{\sigma_1\sigma_2} = (w-z)\langle \Phi^{\bar{z}}_{\sigma_2}, \Phi^w_{\sigma_1}\rangle \qquad \begin{array}{l} \sigma_1,\sigma_2 = \pm \\ z,w \in \rho(H)\cap\rho(H^\Theta) \end{array} \tag{C.32}$$

and satisfying

$$\Gamma^\Theta(z)^* = \Gamma^\Theta(\bar{z}) \tag{C.33}$$

Where * indicates the Hermitian conjugate.
Relation (C.32) does not define univocally matrix Γ^Θ. By direct calculation one can check that the matrix

$$\Gamma^\Theta(z) = \Gamma^0(z) + \Theta \tag{C.34}$$

where Θ is a constant, Hermitian ($\Theta^* = \Theta$), 2×2 matrix and

$$\Gamma^0(z) = \begin{pmatrix} \frac{1}{2i\sqrt{z-\alpha}} & 0 \\ 0 & \frac{1}{2i\sqrt{z+\alpha}} \end{pmatrix} \tag{C.35}$$

satisfies relation (C.32) and (C.33). Different self-adjoint point perturbations of H are parameterized by different choices of the matrix Θ. Being Θ Hermitian H^Θ is a 4-real parameters family of self-adjoint operators.
From the resolvent formula (C.31) it is easily obtained the structure of the domain of H^Θ

$$\begin{aligned} D(H^\Theta) = \Big\{ \Psi \in \mathcal{H}:\ \Psi = \Psi^z + \sum_{\sigma_1,\sigma_2=\pm} (\Gamma^\Theta(z))^{-1}_{\sigma_1\sigma_2}\psi^z_{\sigma_2}(y)\Phi^z_{\sigma_1}; \\ \Psi^z \in D(H),\ \Psi^z = \sum_\sigma \psi^z_\sigma(x)\otimes\chi_\sigma;\ z\in\rho(H)\cap\rho(H^\Theta)\Big\} \end{aligned} \tag{C.36}$$

It is easily seen that if $\Psi \in D(H^\Theta)$ then functions $\psi_\pm(x)$ are continuous but with discontinuous first derivative. Then operators H^Θ belong to the subfamily of δ-like perturbations of H.
If the unitary matrix U_{jk} is parameterized as in (C.25) with $(V_2)_{jk} = \delta_{jk}$, fixed ω, θ, φ and ρ then exists a matrix Θ such that $H^\Theta = H^U$. In general it is not easy to find the correspondence between H^U and H^Θ.

C.2.3 Diagonal δ-like perturbations

A special case in which it is possible to explicitly find the correspondence between H^U and H^Θ is the following.
Consider the unitary matrix

$$U = \begin{pmatrix} U_2 & O_2 \\ O_2 & V_2 \end{pmatrix} \qquad U_2 = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \qquad V_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{C.37}$$

where O_2 is the 2×2 matrix with all zero entries, $\theta \in [0,2\pi]$ and $\varphi \in [0,2\pi]$. We indicate with $\hat{H}$ a self-adjoint operator corresponding to this choice of the unitary matrix and we call "diagonal" the 2-real parameters subfamily $\hat{H}$ because the boundary conditions in y do not mix functions $\psi_+(x)$ and $\psi_-(x)$.

From boundary conditions (C.27) and (C.28) it is easily seen that functions in $D(\hat{H})$ are continuous but have first derivative discontinuous, in formulae

$$D(\hat{H}) = \Big\{\Psi \in \mathcal{H} : \Psi = \sum_{\sigma=\pm} \psi_\sigma(x) \otimes \chi_\sigma;\ \psi_\pm \in H^1(\mathbb{R}) \cap H^2(\mathbb{R}\backslash\{y\}),$$
$$\psi'_\pm(y^+) - \psi'_\pm(y^-) = \gamma_\pm \psi_\pm(y),\ -\infty < \gamma_\pm \leq +\infty\Big\} \tag{C.38}$$

with $\gamma_\pm$ satisfying the relation

$$\gamma_+ = -2\sqrt{1+\alpha^2}\,\frac{\mathrm{Re}\,(e^{-i\theta}\sqrt{\alpha+i}) + \mathrm{Re}\,(\sqrt{\alpha+i})}{\sqrt{1+\alpha^2} - \alpha\cos\theta - \sin\theta} \tag{C.39}$$

$$\gamma_- = 2\sqrt{1+\alpha^2}\,\frac{\mathrm{Im}\,(e^{i\varphi}\sqrt{\alpha+i}) - \mathrm{Im}\,(\sqrt{\alpha+i})}{\sqrt{1+\alpha^2} + \alpha\cos\varphi - \sin\varphi} \tag{C.40}$$

By direct calculation one obtains that the matrix Θ corresponding to (C.37) is $\Theta_{\sigma_1\sigma_2} = \delta_{\sigma_1\sigma_2}(\gamma_{\sigma_1})^{-1}$. In fact the expression of the resolvent corresponding to this choice of the matrix Θ is

$$(\hat{H}-z)^{-1} = (H-z)^{-1} - \sum_{\sigma=\pm} \frac{2\gamma_\sigma\sqrt{z-\sigma\alpha}}{i\gamma_\sigma + 2\sqrt{z-\sigma\alpha}}\langle \Phi^{\bar{z}}_\sigma, \cdot\rangle \Phi^z_\sigma \qquad z \in \rho(\hat{H}) \qquad \mathrm{Im}\,(\sqrt{z\mp\alpha}) > 0 \tag{C.41}$$

and the domain of $\hat{H}$ can be also expressed as

$$D(\hat{H}) = \Big\{\Psi \in \mathcal{H} : \Psi = \Psi^z - \sum_{\sigma=\pm} \frac{2\gamma_\sigma\sqrt{z-\sigma\alpha}}{i\gamma_\sigma + 2\sqrt{z-\sigma\alpha}}\psi^z_\sigma(y)\Phi^z_\sigma;\ \Psi^z \in D(H),$$
$$\Psi^z = \sum_{\sigma=\pm} \psi^z_\sigma(x) \otimes \chi_\sigma;\ -\infty < \gamma_\pm \leq \infty;\ z \in \rho(H) \cap \rho(\hat{H})\Big\} \tag{C.42}$$

The action of $\hat{H}$ on its domain is

$$(\hat{H}-z)\Psi = (H-z)\Psi^z \qquad z \in \rho(H) \cap \rho(\hat{H}) \tag{C.43}$$

C.3 Three dimensions

In dimension three a generic vector in $\mathcal{K}^i$ can be written as

$$\Phi^i = a_1 f_+ + a_2 f_- \qquad \Phi \in \mathcal{K}^i \tag{C.44}$$

where $a_j \in \mathbb{C}$ and the corresponding vector in K^{-i} by U is

$$U\Phi^i = \tilde{a}_1 \tilde{f}_+ + \tilde{a}_2 \tilde{f}_- \tag{C.45}$$

with $\tilde{a}_j = \sum_k U_{jk} a_k$, where U_{jk} is the four dimensional unitary matrix representing the unitary application U in the basis $\{f_+, f_-\}$ and $\{\tilde{f}_+, \tilde{f}_-\}$.
The more general 2×2 unitary matrix has 4 real independent parameters and can be written as

$$U = \begin{pmatrix} e^{i\theta}\cos\omega & e^{i(\theta+\rho)}\sin\omega \\ -e^{i(\varphi-\rho)}\sin\omega & e^{i\varphi}\cos\omega \end{pmatrix} \tag{C.46}$$

where θ, ρ, φ, ω are real parameters. Notice that being, in dimension three, the family of self-adjoint extensions of H_0 parameterized by only four real parameters the unitary matrix (C.46) includes all the possible Hamiltonians that are an extension of H_0.
The generic element in the Hilbert space $\mathcal{H}$ can be written as

$$\Psi = \psi_+(x) \otimes \chi_+ + \psi_-(x) \otimes \chi_- \tag{C.47}$$

In general if $\Psi \in D(H^U)$ functions $\psi_\pm(x)$ have a singularity of order $|x-y|^{-1}$ near y

$$\psi_\pm(x) = \phi_{reg,\pm}(x) + \frac{q_\pm}{4\pi|x-y|} \qquad \phi_{reg,\pm}(x) \in H^2_{loc}(\mathbb{R}^3) \tag{C.48}$$

where $H^2_{loc}(\mathbb{R}^3)$ indicates the homogeneous Sobolev space of locally square-integrable functions with their first and second (distributional) derivative.
Functions $\phi_{reg,\pm}(x)$ are called the regular parts of $\psi_\pm(x)$ and in the following we will refer to $q_\pm$ as charges. Different operators in the family H^U are characterized by a different relation between the values of the regular parts in the point y, $\phi_{reg,\pm}(y)$, and the value of $q_\pm$. By straightforward calculations one obtains that the relation between the charges and $\phi_{reg,\pm}(y)$ is

$$\begin{aligned} q_+ &= c_1\phi_{reg,+}(y) + c_2\phi_{reg,-}(y) \\ q_- &= c_3\phi_{reg,+}(y) + c_4\phi_{reg,-}(y) \end{aligned} \tag{C.49}$$

with

$$\begin{aligned} c_1 &= -4\pi i \frac{(1-e^{i\theta}\cos\omega)(e^{i\varphi}\cos\omega\sqrt{\alpha-i}-\sqrt{\alpha+i}) - e^{i(\theta+\varphi)}\sin^2\omega\sqrt{\alpha-i}}{M} \\ c_2 &= 4\pi\frac{\left\|G^{i+\alpha}\right\|}{\left\|G^{i-\alpha}\right\|}\frac{e^{i(\theta+\rho)}\sin\omega(\sqrt{\alpha-i}-\sqrt{\alpha+i})}{M} \\ c_3 &= 4\pi i\frac{\left\|G^{i-\alpha}\right\|}{\left\|G^{i+\alpha}\right\|}\frac{e^{i(\varphi-\rho)}\sin\omega(\sqrt{\alpha+i}-\sqrt{\alpha-i})}{M} \\ c_4 &= 4\pi\frac{(1-e^{i\varphi}\cos\omega)(e^{i\theta}\cos\omega\sqrt{\alpha+i}+\sqrt{\alpha-i}) - e^{i(\theta+\varphi)}\sin^2\omega\sqrt{\alpha+i}}{M} \end{aligned} \tag{C.50}$$

and

$$\begin{aligned} M = -i\Big[&(e^{i\theta}\cos\omega\sqrt{\alpha+i}+\sqrt{\alpha-i})(e^{i\varphi}\cos\omega\sqrt{\alpha-i}-\sqrt{\alpha+i}) + \\ &- e^{i(\theta+\varphi)}\sin^2\omega\sqrt{1+\alpha^2}\Big] \end{aligned} \tag{C.51}$$

Off-diagonal terms in the matrix U_{jk} are responsible for the coupling between the charge q_+ and the function $\phi_{reg,-}$ and of the coupling between the charge q_- and the function $\phi_{reg,+}$.
Like in dimension one it is possible to use the Krein's formula for the resolvent. It is worth to note that due to dimensionality of the deficiency spaces the 2×2 matrix $\Gamma^\Theta(z)$ completely characterizes all the possible self-adjoint perturbations of H.

Indicating with H^Θ the generic self-adjoint perturbation of the free operator H from formula (A.10) one has

$$(H^\Theta - z)^{-1} = (H-z)^{-1} + \sum_{\sigma_1,\sigma_2=\pm} (\Gamma^\Theta(z))^{-1}_{\sigma_1\sigma_2} \langle \Phi^{\bar{z}}_{\sigma_2}, \cdot \rangle \Phi^z_{\sigma_1} \qquad z \in \rho(H) \cap \rho(H^\Theta) \tag{C.52}$$

Where Φ^z_σ are defined in (C.8) and $\Gamma^\Theta(z)$ is a 2×2 matrix defined in analogy with (C.32) and (C.33).
Like in dimension one by direct evaluation one can check that the matrix $\Gamma^\Theta(z)$ written as

$$\Gamma^\Theta(z) = \Gamma^0(z) + \Theta \tag{C.53}$$

where Θ is a constant, Hermitian ($\Theta^* = \Theta$), 2×2 matrix, and

$$\Gamma^0(z) = \begin{pmatrix} \frac{\sqrt{z-\alpha}}{4\pi i} & 0 \\ 0 & \frac{\sqrt{z+\alpha}}{4\pi i} \end{pmatrix} \tag{C.54}$$

satisfies the analogue of conditions (C.32) and (C.33).
From the resolvent (C.52) it is easy to obtain the domain and the action of H^Θ

$$D(H^\Theta) = \Big\{ \Psi \in \mathcal{H} : \ \Psi = \Psi^z + \sum_{\sigma=\pm} q_\sigma \Phi^z_\sigma; \ \Psi^z \in D(H), \quad \Psi^z = \sum_\sigma \psi^z_\sigma(x) \otimes \chi_\sigma; \ q_\sigma = \sum_{\sigma_1=\pm} (\Gamma^\Theta(z))^{-1}_{\sigma\sigma_1} \psi^z_{\sigma_1}(y); \quad z \in \rho(H) \cap \rho(H^\Theta) \Big\} \tag{C.55}$$

$$(H^\Theta - z)\Psi = (H-z)\Psi^z \qquad z \in \rho(H) \cap \rho(H^\Theta) \tag{C.56}$$

Notice that the charges $q_\pm$ do not depend on z.
Different self-adjoint perturbations of H are characterized by different choices of the matrix Θ and there is a one to one correspondence between the family H^Θ and H^U.
If $H^U = H^\Theta$ functions $\psi^z_\pm$ are related to $\psi_{reg,\pm}$ by

$$\psi^z_\pm(x) = \psi_{reg,\pm}(x) + \frac{q_\pm}{4\pi|x-y|}\left(1 - e^{i\sqrt{z\mp\alpha}|x-y|}\right) \tag{C.57}$$

but in general it is not easy to establish the correspondence between matrices U_{jk} and Θ_{jk}.

C.3.1 Free dynamics, $d = 3$

The simplest self-adjoint extension of H_0 corresponds to choose $\omega = \theta = \varphi = \rho = 0$ in (C.46).
From conditions (C.50) and (C.51) it is easily seen that this choice of the parameters gives $c_1 = c_2 = c_3 = c_4 = 0$. We indicate with H the self-adjoint extension corresponding to this choice of the unitary application U. Functions $\psi_\pm(x)$ in the domain of H have no singularity in $x = y$, then

$$D(H) = H^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \qquad H = -\Delta \otimes \mathbb{I} + \mathbb{I} \otimes \alpha\, \sigma_x \qquad \alpha \in \mathbb{R}. \tag{C.58}$$

H is the generator of the free dynamics in dimension three.

C.3.2 Diagonal perturbations, $d = 3$

The choice $\omega = 0$ in (C.46) corresponds to a very simple case for which it is possible to establish the correspondence between H^U and H^Θ. Like in dimension one we call "diagonal" the subfamily of self-adjoint extensions corresponding to $\omega = 0$. Since for this class it is possible to evaluate explicitly the propagator we discuss it with more detail.
It is a straightforward calculation to check that if $\omega = 0$ conditions (C.50) and (C.51) give

(C.59)

$$\begin{aligned} c_1 &= 4\pi \frac{\mathrm{Re}\,(e^{i\theta}\sqrt{\alpha+i}) - \mathrm{Re}\,(\sqrt{\alpha+i})}{\sqrt{1+\alpha^2} - \alpha\cos\theta + \sin\theta} \\ c_2 &= 0 \\ c_3 &= 0 \\ c_4 &= 4\pi \frac{\mathrm{Im}\,(e^{i\varphi}\sqrt{\alpha-i}) - \mathrm{Im}\,(\sqrt{\alpha-i})}{\sqrt{1+\alpha^2} + \alpha\cos\varphi + \sin\varphi} \end{aligned} \tag{C.60}$$

Consider the matrix $\Theta_{\sigma_j\sigma_k} = \delta_{\sigma_j\sigma_k}\gamma_{\sigma_j}$. We indicate with $\hat{H}$ the Hamiltonian corresponding to this choice of the matrix Θ, $\hat{H}$ is defined by

$$\begin{aligned} D(\hat{H}) = \Big\{ \Psi \in \mathcal{H} : \Psi = \Psi^z + \sum_{\sigma=\pm} \frac{4\pi\psi^z_\sigma(y)}{4\pi\gamma_\sigma - i\sqrt{z-\sigma\alpha}} \Phi^z_\sigma; \\ \Psi^z \in D(H);\ \Psi^z = \sum_\sigma \psi^z_\sigma(x) \otimes \chi_\sigma; \\ -\infty < \gamma_\pm \le \infty\,,\ z \in \rho(\hat{H}) \Big\} \end{aligned} \tag{C.61}$$

$$(\hat{H} - z)\Psi = (H - z)\Psi^z \qquad z \in \rho(H) \cap \rho(\hat{H}) \tag{C.62}$$

To verify that the choice $\omega = 0$ in (C.46) coincides with the operator obtained by $\Theta_{\sigma_j\sigma_k} = \delta_{\sigma_j\sigma_k}\gamma_{\sigma_j}$ suppose that $\Psi \in D(\hat{H})$ and that

$$\Psi = \left(\psi_{reg,+}(x) + \frac{c_1\psi_{reg,+}(y)}{4\pi|x-y|}\right) \otimes \chi_+ \left(\psi_{reg,-}(x) + \frac{c_2\psi_{reg,-}(y)}{4\pi|x-y|}\right) \otimes \chi_- \tag{C.63}$$

The equality

$$\psi_{reg,+}(x) + \frac{c_1\psi_{reg,+}(y)}{4\pi|x-y|} = \psi^z_+(x) + \frac{4\pi\psi^z_+(y)}{4\pi\gamma_+ - i\sqrt{z-\alpha}} \frac{e^{i\sqrt{z-\alpha}|x-y|}}{4\pi|x-y|} \tag{C.64}$$

holds if $\gamma_+ = (c_1)^{-1}$. The analogous equality for the χ_--part of Ψ holds if $\gamma_- = (c_2)^{-1}$. The operator $\hat{H}$ has the same domain of the operator corresponding to the choice $\omega = 0$ then the two operators coincide.

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