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**Models of few (and many) body
quantum systems with Point
Interactions**

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Preface

A series of international conferences on foundation of Quantum Mechanics held in the last years all over Europe were titled “Quantum Theory without Collapse”. The title expresses well a main aspect and a widespread presumption common to a series of scientific programs that, since the sixties of last century, investigated the border between Classical and Quantum Mechanics.

Since then, Experimental Physics explored in various ways the possibility of building up larger and larger systems (with respect to the atomic scale) still showing a quantum behavior. At the same time many theoreticians examined the onset of classicality in quantum systems or made available quantum models of macroscopic measurement apparatus. All these achievements were essential in the formulation of Quantum Information Theory and in the search for hardware and software of the future quantum computer.

All those attempts share the belief that a reduction of Classical Mechanics to Quantum Theory is somehow possible and tend to analyze the dynamics of the quantum-to-classical transition. This point of view is in flat contradiction with the postulate of “collapse of the wave packet” which ratifies an explicit renounce to any reduction program stating the validity of different dynamical laws at different length scales. In spite of a growing number of scientists working on different aspects of the reduction program, the difficulties of bridging the classical and the quantum world became clearer only recently.

The situation outlined above is in fact reminiscent of the Boltzmann program of reduction of the thermodynamical laws to classical dynamics. Analogies are made closer by the fact that often, in the recent literature, decoherence phenomena in quantum systems are described in thermodynamical terms through concepts like quantum information entropies or the irreversible diffusion of entanglement induced by the interaction with macroscopic systems. It happens that after more than a century the Boltzmann program is still in progress. Almost every scientist believe in the existence of a mechanical explanation of the second law of Thermodynamics but, up to now, not a single mechanical model where the second law is deduced or simply investigated in dynamical terms is available. There are no reasons to believe that results will come quicker in the reduction program of Classical Mechanics to Quantum Theory. In both fields different methodologies were used in various attempts to un-

derstand the behavior of many-component dynamical systems: analysis of the consequences of statistical assumptions on the elementary interaction events, qualitative theory of dynamical systems, constructive approaches based on the analysis of simple models of the physical systems under study and many others.

The work presented in this thesis is fully inside the last category mentioned above. Our aim is to make available models of multipartite quantum systems which are simple enough to be analytically approachable, but showing characteristic features of more complex systems. The main technical tool we rely on is the theory of point interaction Hamiltonians which will be generalized in this thesis to multipartite systems.

In the first two chapters we present a brief outline of the theory of open quantum systems and few particular developments in the so called “decoherence program”. It will be stressed that this kind of results either do not give much insight in the transition quantum-classical or require assumptions almost impossible to be “rigorously” justified.

In the rest of the thesis we will try to support our opinion that more detailed instances about large quantum systems can only be inferred analyzing simple models of quantum systems showing non trivial dynamics.

Point interaction Hamiltonians have been the building blocks of any model presented in this thesis work.

Since the early days of Quantum Mechanics zero range quantum interactions revealed an undoubted effectiveness whenever solvability together with non triviality was required. In chapter 3 and in appendix B, we give an introduction to point interaction Hamiltonians.

In chapter four the decoherence effects induced by scattering events are analyzed. In this framework we study a rigorous derivation of a well known empirical formula for the evolution of a quantum system composed by two particles with a small mass ratio, the *Joos and Zeh formula*. The estimates obtained are subsequently used to evaluate the effects of decoherence induced by the interaction.

In chapter five we analyze the dynamics of a quantum particle in an array of localized spins interacting via point potentials depending on the state of the spins. Our main interest is to define a model of a the tracking chamber, that we investigate in detail in chapter six. The mathematical features of this model allow us to show that, because of the interaction with the spins, the reduced density matrix relative to the particle, initially in a pure state, evolves dynamically in a statistical mixture.

Interchanging the role of system and environment with respect to the model of a tracking chamber we can think of a model-atom, a localized quantum system with a finite number of energy states, interacting with a gas of (non interacting) particles. Popular wisdom suggests that, if the interaction with the gas is switched on, only few eigenstates of the atom including the ground state

remain stable. The most well-known physical system showing this behavior is the one formed by an atom in the radiation field. Phenomenology suggests that the excited states of the atom decay with spontaneous emission into the ground state. Such kind of results are very difficult to be deduced from the Hamiltonian of the whole system in realistic cases. We construct a model where this mechanism is easy to analyze both qualitatively and quantitatively. In spite of their simplicity the Hamiltonians we define show interesting spectral features considered to be typical of more complex and realistic systems. In our model we show explicitly that the appearance of metastable states comes as a perturbation of spectra where eigenstates embedded in the continuous part of the spectrum are present.

Part I

Models of open quantum systems

Chapter 1

The general approach to open quantum systems

Quantum theory was originally developed to give an explanation of the energy levels of electrons in atoms and of the wave-like behavior of beams of particles in diffraction experiments. Very accurate results were given in terms of the dynamics of one-particle systems. As in Classical Mechanics, detailed perturbation procedures were formulated in order to compute corrections to the one-body dynamics induced by small interactions with other particles.

Nature and consequences of the interaction between a microscopic system and a macroscopic one and the investigation of the effective boundary between the microscopic and the macroscopic world were ruled out by means of few axioms stating, in short, that the two worlds were governed by different dynamical laws and that microscopic systems undergo sudden and stochastic changes when interacting with macroscopic ones.

Only later an effort has been made to characterize general features of the behavior of a quantum system in continuous presence of a large environment about which only a limited statistical knowledge is available. The general framework for this field of investigations is usually referred to as the theory of quantum open systems.

Intimately connected with the theory of open quantum systems [17] is the so called decoherence phenomenon, the irreversible migration of quantum correlations to the environment and the consequent more classical behavior of a quantum system.

In this chapter we outline some notation and main results in the theory of open quantum systems. In particular we will review few general statements about the reduced dynamics of a microscopic quantum system in interaction with a complex environment.

1.1 Open quantum systems: the role of the environment

Let S be a quantum system and \mathcal{H} the Hilbert space of its pure states. A vector state $|\psi(t)\rangle \in \mathcal{H}$ contains the maximal kinematical knowledge one can have at time t about the system. According to the postulates of quantum mechanics we know that this state evolves according to Schrödinger's equation (in units $\hbar = m = 1$)

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (1.1)$$

As it is well known, under suitable assumptions on the family of self-adjoint operators $H(t)$, (1.1) admits a unique solution specified by a unitary flow $U(t, t_0)$ which connect the state at the time t_0 to the state $|\psi(t)\rangle$ at a generic time t

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle \quad (1.2)$$

If we consider an isolated physical system the selfadjoint Hamiltonian H is time independent and the evolution operator can be written as

$$U(t, t_0) = e^{-iH(t-t_0)} \quad (1.3)$$

which always exists by Stone's theorem. For a time dependent Hamiltonian this operator assumes the formal expression

$$\begin{aligned} U(t, t_0) &= \left(\mathbb{I} + \sum_{n=1}^{\infty} (-i)^n \int_s^t dt_1 \dots \int_s^{t_{n-1}} dt_n H(t_1) \dots H(t_n) \right) \\ &= T_{\leftarrow} e^{-i \int_{t_0}^t ds H(s)} \end{aligned} \quad (1.4)$$

where T_{\leftarrow} is the chronological time-ordering operator¹. Formula (1.4) is a *formal* definition in the sense that the corresponding series expansion is convergent for small times if the $H(t)$ are uniformly bounded and it is often not even defined term by term in the generic case of unbounded Hamiltonians.

In general the initial state of a quantum system is a mixed state, described by the density operator ρ .

It is worth recalling some fundamental properties of this operator:

i) ρ is an hermitian trace-class operator

ii) ρ is non negative :

$$\langle \psi | \rho | \psi \rangle \geq 0 \quad \forall \psi \in \mathcal{H}$$

¹this operator orders products of time-dependent operators in such a way that their time-arguments increase from right to left

iii) ρ has unitary trace.

$$\text{Tr}(\rho) = 1 \quad (1.5)$$

iv) for every basis in \mathcal{H} all the diagonal elements of ρ are non negative. In particular the eigenvalues are all non negative.

v) the trace of ρ^2 satisfies $\text{tr}(\rho^2) \leq 1$; the equal sign holds true only when ρ is a projection operator $|\psi\rangle\langle\psi|$ which means that the system is in the pure state $|\psi\rangle$.

From the postulates of quantum mechanics, when the state of a quantum system is described by a density matrix ρ , the probability of obtaining the value λ in the subset $\Delta \subseteq \mathbb{R}$, when measuring observable A (which will be identified here with the corresponding self adjoint operator), is

$$P_{A,\rho}(\Delta) = \text{tr}(\rho\Pi_A(\Delta))$$

where $\Pi_A(\Delta)$ is the spectral projector on Δ of the operator A .

The density operator at time t is given by

$$\rho(t) = U(t, t_0)\rho(t_0)U^\dagger(t, t_0) \quad (1.6)$$

where $\rho(t_0)$ is the density operator at time t_0 and $U(t, t_0)$ is the evolution operator. Deriving with respect to t both sides of (1.6) we obtain the equation of motion for $\rho(t)$, called the *Liouville-von Neumann equation*

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)] = \mathcal{L}(t)\rho(t) \quad (1.7)$$

The formal solution of (1.7) can be written as

$$\rho(t) = T_{\leftarrow} \exp \left[\int_{t_0}^t ds \mathcal{L}(s) \right] \rho(t_0) \quad (1.8)$$

If we consider a system S in interaction with a system B we have to consider the composite quantum system $S + B$.

Suppose that S and B are two quantum systems distinguishable for every t , described respectively in the Hilbert spaces \mathcal{H}_S and \mathcal{H}_B . The total Hilbert space \mathcal{H} is given by the tensor product

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B \quad (1.9)$$

with elements (φ, ψ) such that $\varphi \in \mathcal{H}_S$ and $\psi \in \mathcal{H}_B$ linear both in the first and in the second component:

$$\begin{aligned}
& \forall \alpha, \beta \in \mathbb{C}, \forall \psi, \phi \in \mathcal{H}_S \quad \forall \varphi, \chi \in \mathcal{H}_B \\
& (\alpha\psi + \beta\phi) \otimes \chi = (\alpha\psi) \otimes \chi + (\beta\phi) \otimes \chi \\
& \psi \otimes (\alpha\varphi + \beta\chi) = \psi \otimes (\alpha\varphi) + \psi \otimes (\beta\chi)
\end{aligned} \tag{1.10}$$

Consider two basis $\{|\varphi_i^{(S)}\rangle\}$ e $\{|\varphi_j^{(B)}\rangle\}$ respectively in \mathcal{H}_S e \mathcal{H}_B .

The vectors $|\varphi_i^{(S)}\rangle \otimes |\varphi_j^{(B)}\rangle$ are a basis for \mathcal{H} , so that a generic vector in \mathcal{H} can be written as

$$|\Psi\rangle = \sum_{i,j} \alpha_{i,j} |\varphi_i^{(S)}\rangle \otimes |\varphi_j^{(B)}\rangle \tag{1.11}$$

If $A^{(S)}$ is an operator acting on $\mathcal{H}^{(S)}$ and $A^{(B)}$ on $\mathcal{H}^{(B)}$, the tensor product $A^{(S)} \otimes A^{(B)}$ is defined as

$$(A^{(S)} \otimes A^{(B)})(|\varphi_i^{(S)}\rangle \otimes |\varphi_j^{(B)}\rangle) = (A^{(S)}|\varphi_i^{(S)}\rangle) \otimes (A^{(B)}|\varphi_j^{(B)}\rangle) \tag{1.12}$$

and in this way it is possible to obtain the action of this operator on a generic vector in $\mathcal{H}_S \otimes \mathcal{H}_B$. Observables in S are associated with operators of the form $A^{(S)} \otimes I^{(B)}$ and observables in B with operators $I^{(S)} \otimes A^{(B)}$, where with $I^{(S)}$ and $I^{(B)}$ we have indicated the identity operators respectively in \mathcal{H}_S and \mathcal{H}_B .

We indicate with ρ the density matrix for the total system $S + B$. If we are interested only on observables $A^{(S)}$ for the subsystem S notice that

$$\begin{aligned}
\langle A^{(S)} \rangle &= \text{tr} [(A^{(S)} \otimes \mathbb{I}^{(B)}) \rho] \\
&= \sum_{i,j} (\langle \varphi_i^{(S)} | \otimes \langle \chi_j^{(B)} |) (A^{(S)} \otimes \mathbb{I}^{(B)}) \rho (|\varphi_i^{(S)}\rangle \otimes |\chi_j^{(B)}\rangle) = \\
&= \sum_i \langle \varphi_i^{(S)} | \otimes A^{(S)} \sum_j \langle \chi_j^{(B)} | \rho (|\varphi_i^{(S)}\rangle \otimes |\chi_j^{(B)}\rangle) = \\
&= \sum_i \langle \varphi_i^{(S)} | A^{(S)} \rho_S | \varphi_i^{(S)} \rangle = \\
&= \text{tr}_S [A^{(S)} \rho_S]
\end{aligned}$$

where we have defined $\rho_S = \text{tr}_B \rho = \sum_j \langle \chi_j^{(B)} | \rho | \chi_j^{(B)} \rangle$, the partial trace with respect to the subsystem B .

The reduced density matrix evolves according to the equation

$$\rho_S(t) = \text{tr}_B \{U(t, t_0) \rho(t_0) U^\dagger(t, t_0)\} \tag{1.13}$$

where $U(t, t_0)$ is the time evolution operator of the total system.

Deriving with respect to time we get

$$\frac{d}{dt} \rho_S(t) = -i \text{tr}_B [H(t), \rho(t)] \tag{1.14}$$

which still contains the total Hamiltonian as well as the density matrix of the whole system ρ .

1.1.1 The dynamical map

We are interested in the dynamical evolution of the subsystem S . For this purpose we introduce now the notion of *dynamical map*. Let us suppose that at time $t = 0$ the states of S and B are not correlated, in such a way that the initial state of the total system $S + B$ takes the form $\rho(0) = \rho_S(0) \otimes \rho_B(0)$, where $\rho_S(0)$ is the initial state of the system S and $\rho_B(0)$ represents the initial state of the environment.

The construction of the dynamical map is based on the following scheme:

$$\boxed{
 \begin{array}{ccc}
 \rho(0) = \rho_S(0) \otimes \rho_B & \xrightarrow{\text{unitary evolution}} & \rho(t) = U(t, 0) [\rho_S(0) \otimes \rho_B] U^\dagger(t, 0) \\
 \text{tr}_B \downarrow & & \downarrow \text{tr}_B \\
 \rho_S(0) & \xrightarrow{\text{dynamical map}} & \rho_S(t) = V(t) \rho_S(0)
 \end{array}
 } \quad (1.15)$$

The action of the dynamical map is the following:

$$\rho_S(0) \mapsto \rho_S(t) = V(t) \rho_S(0) \equiv \text{tr}_B \{ U(t, 0) [\rho_S \otimes \rho_B] U^\dagger(t, 0) \} \quad (1.16)$$

The reduced density matrix $\rho_S(t)$ at time t can be obtained tracing over the degrees of freedom of the system B the density matrix for the total system ρ . It is worth stressing that (1.14) and (1.16) are not evolution equations for the dynamical map. From a formal point of view this is clear from the fact that the two formulas still contain $U(t, 0)$ which specifies the overall evolution of system and environment. The specific form of the influence of the environment on the system obviously depends on the initial state and on the real evolution of the environment up to time t .

The theory of open quantum systems analyzes the physical situations in which it is possible to assume some a priori form of the dynamical map.

The most well known achievements of the theory refer to the so called Markovian limit, where, in short, it is assumed that the effect on the system at time t is generically independent from the past evolution of the environment but only depends on its state at time t . We will come back on the justification of the Markovian assumption in the next sections. A consequence of the assumption is that the dynamical map has the semigroup property:

$$V(t_1)V(t_2) = V(t_1 + t_2) \quad t_1, t_2 \geq 0 \quad (1.17)$$

which means that the dynamics of the subsystem S can be described using a generator for the time evolution.

Before starting the analysis of the Markovian case we want to write down a new expression for the dynamical map. If we choose an orthonormal basis in \mathcal{H}_B with vectors $|\phi_\alpha\rangle$ and assume that the state of the environment can be given in the form

$$\rho_B = \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}| \quad (1.18)$$

with λ_α non negative real numbers such that $\sum_\alpha \lambda_\alpha = 1$.

From the definition of dynamical map (1.16) it follows that the action of $V(t)$ is

$$V(t)\rho_S = \sum_{\alpha,\beta} W_{\alpha,\beta}(t)\rho_S W_{\alpha,\beta}^\dagger(t) \quad (1.19)$$

if $W_{\alpha,\beta}(t)$ are operators in \mathcal{H}_S defined as

$$W_{\alpha,\beta}(t) = \sqrt{\lambda_\beta} \langle \phi_\alpha | U(t, 0) | \phi_\beta \rangle \quad (1.20)$$

satisfying the following condition

$$\sum_{\alpha,\beta} W_{\alpha\beta}^\dagger W_{\alpha\beta} = I_S \quad (1.21)$$

Notice that the operators $W_{\alpha,\beta}(t)$ are written in terms of the operator $U(t, 0)$ so that (1.19) is not a closed equation for ρ_S for the same reasons mentioned before. In the next section we analyze the structure of the dynamical map if the condition (1.17) is satisfied; then we shortly describe the conditions under which we can justify (1.17).

1.1.2 The Markovian quantum master equation

If the condition (1.17) is satisfied then it exists a generator \mathcal{L} such that

$$V(t) = \exp(\mathcal{L}t) \quad (1.22)$$

and the dynamics of the reduced density matrix for the system S is governed by the differential equation

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t) \quad (1.23)$$

which is known as the *quantum master equation*.

The action of the generator \mathcal{L} was derived in the case of a finite dimensional Hilbert space by Gorini, Kossakowski and Sudarshan in 1976 (see [49]). In the following we recall some of their results without a detailed mathematical derivation (for a complete list of references and an exhaustive treatment see [21]).

Given some Hilbert space \mathcal{H} the Liouville space \mathbf{L} is the space of Hilbert-Schmidt operators A in \mathcal{H} for which $\text{tr}(A^\dagger A)$ is finite. Equipped with the scalar product $(A, B) \equiv \text{tr}\{A^\dagger B\}$ \mathbf{L} becomes a Hilbert space and we can therefore introduce an orthonormal basis in \mathbf{L} satisfying the orthogonality and the completeness conditions.

For the sake of simplicity, let us consider the case when \mathcal{H}_S has finite dimension N . We are able to choose a basis of orthonormal operators F_i with $i = 1, 2, \dots, N^2$ of the corresponding Liouville complex space, such that

$$(F_i, F_j) \equiv \text{tr}_S \{F_i^\dagger F_j\} = \delta_{ij} \quad (1.24)$$

With this definition we can decompose operator in (1.19) as:

$$W_{\alpha\beta}(t) = \sum_{i=1}^{N^2} (F_i, W_{\alpha\beta}(t)) F_i \quad (1.25)$$

and we can rewrite the dynamical map as

$$V(t)\rho_S = \sum_{i,j=1}^{N^2} c_{ij}(t) F_i \rho_S F_j^\dagger \quad c_{ij}(t) \equiv \sum_{\alpha,\beta} (F_i, W_{\alpha\beta}(t)) (F_j, W_{\alpha\beta}(t))^* \quad (1.26)$$

where the coefficient matrix (c_{ij}) is hermitian and positive.

From the definition (1.23) of \mathcal{L} :

$$\mathcal{L}\rho_S = \lim_{\epsilon \rightarrow 0} \{V(\epsilon)\rho_S - \rho_S\} \quad (1.27)$$

and with the further definitions

$$\begin{aligned} a_{ij} &= \lim_{\epsilon \rightarrow 0} \frac{c_{ij}(\epsilon)}{\epsilon} & a_{N^2 N^2} &= \lim_{\epsilon \rightarrow 0} \frac{c_{N^2 N^2}(\epsilon) - N}{\epsilon} \\ F &= \frac{1}{\sqrt{N}} \sum_{i=1}^{N^2-1} a_{i N^2} F_i & G &= -\frac{1}{2} \sum_{i,j=1}^{N^2-1} a_{ij} F_j^\dagger F_i \end{aligned} \quad (1.28)$$

one can derive the *first standard form*

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{i,j=1}^{N^2-1} a_{ij} \left(F_i \rho_S F_j^\dagger - \frac{1}{2} \{F_j^\dagger F_i, \rho_S\} \right) \quad (1.29)$$

The coefficient matrix (a_{ij}) is positive and may be diagonalized

$$u a u^\dagger = \begin{pmatrix} \gamma_1 & 0 & 0 & 0 & 0 \\ 0 & \gamma_2 & 0 & 0 & 0 \\ 0 & 0 & \cdot & 0 & 0 \\ 0 & 0 & 0 & \cdot & 0 \\ 0 & 0 & 0 & 0 & \gamma_{N^2-1} \end{pmatrix} \quad \gamma_i \geq 0 \quad (1.30)$$

Defining a new set of operators A_k through

$$F_i = \sum_{k=1}^{N^2-1} u_{ki} A_k \quad (1.31)$$

one can obtain the diagonal form of the operator \mathcal{L} :

$$\mathcal{L}\rho_S = -i[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left[A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right] \quad (1.32)$$

This is the most general form for the generator: the first term in (1.32) is the unitary part of the dynamics generated by the Hamiltonian H while the second part is usually called *the dissipator*

$$\mathcal{D}(\rho_S) \equiv \sum_{k=1}^{N^2-1} \gamma_k \left[A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right] \quad (1.33)$$

where γ_k has the dimensions of the inverse of a time.

1.1.3 Derivation of the generator for a quantum dynamical semi-group

In the previous section we have analyzed the structure of the generator of a quantum dynamical semigroup. In this section we want to analyze the physical approximation justifying this kind of equation starting from the Hamiltonian H for the total system.

Let us start rewriting the total Hamiltonian as

$$H = H_S + H_B + \hat{H}_I \quad (1.34)$$

where

H_S is the Hamiltonian of the system

H_B is the Hamiltonian of the environment

\hat{H}_I is the Hamiltonian of the interaction between S and B

We can adopt now the point of view of the interaction picture in the description of the dynamical evolution of the density matrix for the total system.

Let us recall briefly that the interaction picture is based on the following decomposition

$$H(t) = H_0 + \hat{H}_I(t) \quad (1.35)$$

where H_0 is the Hamiltonian when the interaction between the systems is ignored, while $\hat{H}_I(t)$ is the Hamiltonian describing the interaction. The time evolution operator of the total system will be again denoted by $U(t, t_0)$ and the expectation value of a Schrödinger observable $A(t)$ (which may depend explicitly on time) at time t is given by

$$\langle A(t) \rangle = \text{tr}(A(t)U(t, t_0)\rho(t_0)U^\dagger(t, t_0)) \quad (1.36)$$

where $\rho(t_0)$ is the state of the whole system at time t_0 . Let us define the unitary time evolution operators

$$U_0(t, t_0) \equiv e^{-iH_0(t-t_0)} \quad (1.37)$$

and

$$U_I(t, t_0) \equiv U_0^\dagger(t, t_0)U(t, t_0) \quad (1.38)$$

Then the (1.36) may be written as

$$\langle A(t) \rangle = \text{tr} \left\{ U_0^\dagger(t, t_0)A(t)U_0(t, t_0)U_I(t, t_0)\rho(t_0)U_I^\dagger(t, t_0) \right\} \equiv \text{tr} \{ A_I(t)\rho_I(t) \}$$

where

$$A_I(t) \equiv U_0^\dagger(t, t_0)A(t)U_0(t, t_0)$$

and

$$\rho_I(t) \equiv U_I(t, t_0)\rho(t_0)U_I^\dagger(t, t_0)$$

The operator $U_I(t, t_0)$ is the solution of the equation

$$i\frac{\partial}{\partial t}U_I(t, t_0) = H_I(t)U_I(t, t_0)$$

subject to the initial condition $U_I(t, t_0) = \mathbb{I}$ and where $H_I(t)$ is the Hamiltonian in the interaction picture

$$H_I(t) \equiv U_0^\dagger(t, t_0)\hat{H}_I(t)U_0(t, t_0)$$

One can be easily obtain that

$$\frac{d}{dt}\rho(t) = -i[H_I(t), \rho(t)] \quad (1.39)$$

whose formal solution can be written as

$$\rho(t) = \rho(0) - i \int_0^t ds [H_I(s), \rho(s)] \quad (1.40)$$

We perform the trace over the degrees of freedom of the environment B in (1.39), assume $\text{tr}_B [H_I(t), \rho(0)] = 0$ and substitute in (1.39) in order to obtain

$$\frac{d}{dt}\rho_S(t) = - \int_0^t ds \text{tr}_B [H_I(t), [H_I(s), \rho(s)]] \quad (1.41)$$

At the first step we have to eliminate $\rho(t)$ in the right side because we want to write an equation only for the reduced density matrix relative to the system. The first physical assumption needed is the validity of the *Born approximation* which is based on the hypothesis that the coupling between S and B is weak and the state of B changes very slowly.

In this case the reduced density matrix for the environment is not affected by the interaction

$$\rho(t) \approx \rho_S(t) \otimes \rho_B \quad (1.42)$$

Equation (1.41) becomes

$$\frac{d}{dt}\rho_S(t) = - \int_0^t ds \operatorname{tr}_B [H_I(t), [H_I(s)\rho_S(s) \otimes \rho_B]] \quad (1.43)$$

At the second step we want to substitute $\rho(s)$ in the integrand with $\rho(t)$ in order to obtain an equation of motion for the reduced density matrix in which the time evolution of the state at time t depends only by the state of the system at the same time. This is the core approximation and takes the name of *Markov approximation*.

With this assumption, equation (1.43) becomes local in time

$$\frac{d}{dt}\rho_S(t) = - \int_0^t ds \operatorname{tr}_B [H_I(t), [H_I(s)\rho_S(t) \otimes \rho_B]] \quad (1.44)$$

The Markovian approximation is not conclusive because (1.44) still shows an explicit dependence on the initial condition. If we can replace s with $t - s$ and if we can put the upper limit of integration to infinity equation (1.44) shows a true Markovian behavior. The physical assumption in order to achieve this mathematical condition is the following: the time scale τ_R of variability relative to the system S is very large if compared with the time of decay τ_B over which the correlations functions of the environment decay, i.e. $\tau_B \ll \tau_R$.

With all the approximations discussed before we obtain:

$$\frac{d}{dt}\rho_S(t) = - \int_0^\infty ds \operatorname{tr}_B [H_I(t), [H_I(t - s)\rho_S(t) \otimes \rho_B]] \quad (1.45)$$

In general it is not true that starting from (1.45) is possible to derive and write a dynamical semigroup. With another approximation, known as *rotating wave approximation*, we can finally recover the first standard form.

To explain this approximation consider the most general form of the Hamiltonian H_I

$$H_I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha} \quad A_{\alpha}^{\dagger} = A_{\alpha} \quad B_{\alpha}^{\dagger} = B_{\alpha} \quad (1.46)$$

and suppose that the spectrum of the Hamiltonian H_S is discrete with eigenvalues ϵ_i and projectors into the eigenspaces $\Pi(\epsilon_i)$. Then the operators A_{α} can be written as

$$A_{\alpha}(\omega) \equiv \sum_{\epsilon_j - \epsilon_i = \omega} \Pi(\epsilon_i) A_{\alpha} \Pi(\epsilon_j) \quad (1.47)$$

where the sum is over all energy eigenvalues ϵ_i and ϵ_j with a fixed energy gap ω . The following relations are satisfied

$$\begin{aligned} [H_S, A_\alpha(\omega)] &= -\omega A_\alpha(\omega) \mapsto e^{-iH_S t} A_\alpha(\omega) e^{-iH_S t} = e^{-i\omega t} A_\alpha(\omega) \\ [H_S, A_\alpha^\dagger(\omega)] &= \omega A_\alpha^\dagger(\omega) \mapsto e^{-iH_S t} A_\alpha^\dagger(\omega) e^{-iH_S t} = e^{i\omega t} A_\alpha^\dagger(\omega) \end{aligned} \quad (1.48)$$

and it can be easily verified that

$$[H_S, A_\alpha^\dagger(\omega) A_\beta(\omega)] = 0$$

$$A_\alpha^\dagger(\omega) = A_\alpha(-\omega)$$

The operator A_α can be written as

$$\sum_{\omega} A_\alpha(\omega) = \sum_{\omega} A_\alpha^\dagger(\omega) = A_\alpha \quad (1.49)$$

and the Hamiltonian $H_I(t)$ assumes the expression

$$H_I(t) = \sum_{\alpha, \omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha(t) \quad B_\alpha(t) = e^{iH_B t} B_\alpha e^{-iH_B t} \quad (1.50)$$

We can now substitute (1.50) into (1.45) and obtain

$$\frac{d}{dt} \rho_S(t) = \sum_{\omega, \omega'} \sum_{\alpha, \beta} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) (A_\beta(\omega) \rho_S(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_S(t)) + \text{h.c.} \quad (1.51)$$

where h.c. means hermitian conjugate and

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle$$

is the one-sided Fourier transform of the reservoir correlation function

$$\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle$$

If the state of the environment ρ_B is stationary, $[H_B, \rho_B] = 0$ and then the correlations are homogeneous in time $\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle = \langle B_\alpha^\dagger(s) B_\beta(0) \rangle$ and $\Gamma_{\alpha\beta}(\omega)$ is time independent.

The approximation of the rotating wave consists in an operation of averaging over the rapid oscillations terms in (1.51). Let τ_S be the typical time scale of the intrinsic evolution of the system S , defined by a typical value $|\omega - \omega'|^{-1}$ ($\omega' \neq \omega$) and τ_R is the relaxation time for the environment. The assumption related to this approximation is that the condition $\tau_S \gg \tau_R$ is satisfied. Then all the terms in (1.51) with $\omega \neq \omega'$ can be neglected because they produce very rapid oscillations during the time in which ρ_S varies appreciably.

Finally, with the following position

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + iS_{\alpha\beta}(\omega)$$

we obtain the first standard form for the master equation

$$\frac{d}{dt}\rho_S(t) = -i[H_{LS}, \rho_S(t)] + \mathcal{D}(\rho_S(t)) \quad (1.52)$$

where

$$H_{LS} = \sum_{\omega} \sum_{\alpha,\beta} S_{\alpha\beta}(\omega) A_{\alpha}^{\dagger}(\omega) A_{\beta}(\omega)$$

is usually called Lamb shift Hamiltonian since it leads to a renormalization of the unperturbed energy of H_S induced by the interaction and

$$\mathcal{D}(\rho_S(t)) = \sum_{\omega} \sum_{\alpha,\beta} \gamma_{\alpha\beta}(\omega) \left(A_{\beta}(\omega) \rho_S(t) A_{\alpha}^{\dagger}(\omega') - \frac{1}{2} \{ A_{\alpha}^{\dagger}(\omega') A_{\beta}(\omega), \rho_S(t) \} \right)$$

is the dissipator.

Performing a diagonalization of $\gamma_{\alpha\beta}(\omega)$ we can recover the second standard form (1.32) for the master equation.

Chapter 2

Decoherence

2.1 The program of decoherence

Apart from few seminal contribution, often completely outside the current mainstream, it was only around the 80's of the last century that decoherence theory was formulated in a clear way in some very important works (see e.g. [46] for an updated list of references), starting one of the most interesting debate in fundamental quantum mechanics.

In this paragraph we analyze some preliminary aspects of decoherence theory and the connection of this phenomenon with the quantum measurement problem.

The “decoherence program” is based on a fundamental hypothesis: in presence of even a weak interaction between a quantum system and the surrounding environment, the quantum correlations spread very quickly over the degrees of freedom of the environment. The observables relative to any subsystem become rapidly more classical, while the only quantities that preserve a quantum behavior are collective variables more and more out of reach for any observation.

Decoherence theory remains of course inside the frame of the general theory of quantum open systems with two main peculiar features:

- an attempt is made to characterize qualitatively and quantitatively the specific quantum environment under investigation;
- the reduced dynamics is analyzed in terms of the “degree of classicality” induced on the system by the interaction with the environment or the measurement apparatus

The decoherence program took different directions of research which can roughly be classified according to their degree of generality.

A line of research faced fundamental problems about the way the interaction with a macroscopic apparatus picks up a definite orthonormal basis of states

and the way decoherence can be quantified by the suppression of interference terms.

A second approach has been characterized by the search for statistical models of the environment. In general a detailed analysis of the response of the one-body dynamics to the interaction with the environment together with some classical reasoning about the statistics of the interaction brought to tentative master equations typical of the physical settings of the model.

A third attempt is based on a detailed analysis of the Schrödinger dynamics of system and environment. It is a bottom-up approach that requires the availability of simple models of multipartite systems, where simple means, in this context, that results about the exact dynamics are analytically attainable.

In this chapter we will only mention the main ideas behind the first approach and few results about the phenomenon of decoherence induced by scattering investigated with methods typical of the second approach. In the rest of the thesis we will discuss methods based on the use of solvable models of environment.

2.1.1 Mechanism of superselection

In this section we give a standard introduction to the decoherence program. We first outline some controversial facts in the so called ideal measuring process of von Neumann and we clarify the way in which the decoherence program attempts to overcome the problem.

In the interpretative scheme of the decoherence program one *“key idea”* is that in every measuring process there are three systems: the system S , the measuring apparatus A and an environment E surrounding them.

In the following we indicate the state of the system, of the apparatus and of the environment respectively with $|s_n\rangle$, $|a_n\rangle$ and $|e_n\rangle$.

The total Hilbert space is:

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_S \otimes \mathcal{H}_A \otimes \mathcal{H}_E$$

The von Neumann scheme is a concise form of an intuitive approach to a description of a measuring process:

$$\begin{aligned} \left(\sum_n c_n |s_n\rangle \right) \otimes |a_r\rangle \otimes |e_0\rangle &\xrightarrow{\text{interaction } S+A} \left(\sum_n c_n |s_n\rangle \otimes |a_n\rangle \right) \otimes |e_0\rangle \\ &\xrightarrow{\text{interaction } S+A+E} \sum_n c_n |s_n\rangle \otimes |a_n\rangle \otimes |e_n\rangle \end{aligned} \quad (2.1)$$

We recall that by the biorthogonal decomposition theorem, given a state $|\psi\rangle$ of the composite system $\mathcal{H}_S \otimes \mathcal{H}_A$, there exist bases $\{|s_n\rangle\}$ in \mathcal{H}_S and $\{|a_n\rangle\}$ in \mathcal{H}_A such that this state can be written as a linear combination of vectors of

the form $|s_n\rangle \otimes |a_n\rangle$. If the absolute values (modulus) of the coefficients in this linear combination are all unequal then the basis is unique.

In general the state a $\mathcal{A} + \mathcal{S}$ can be written in more than one way. For example

$$|\psi\rangle = \sum_n c_n |s_n\rangle \otimes |a_n\rangle$$

and

$$|\psi\rangle = \sum_n c'_n |s'_n\rangle \otimes |a'_n\rangle$$

with $|a_n\rangle$ and $|a'_n\rangle$ well distinguished states, which means that there are no phase factors α_n such that $|a'_n\rangle = e^{i\alpha_n} |a_n\rangle$.

Suppose we have two measuring apparatus A , suitable for measuring the observables $A = \sum_n \lambda_n |s_n\rangle \langle s_n|$ and $B = \sum_n \lambda'_n |s'_n\rangle \langle s'_n|$. Without any further hypothesis about the commutation relation between these observables it is possible to perform together the two measurements.

If the whole system is made up of three subsystems \mathcal{A} , \mathcal{S} and \mathcal{E} , the tridecompositional uniqueness theorem ([70]) guarantees that if a Schmidt decomposition $|\psi\rangle = \sum_n c_n |s_n\rangle \otimes |a_n\rangle \otimes |e_n\rangle$ exists, then it is unique. Notice that unlike the bipartite system case the decomposition might not exist.

Given any pure state in the whole Hilbert space \mathcal{H}_{tot} neither we know whether a Schmidt decomposition exists nor we are given the unique expansion itself (provided that the decomposition exists).

Additional criterions are needed then to determine what are the basis of the apparatus (the preferred pointer states) for a “faithful measurement”.

The idea is that these criterions can be searched looking at the interaction in terms of preservation and robustness of the correlations. Until now we have assumed that the interaction with the environment does not disturb the correlation between the state of system \mathcal{S} , $|s_n\rangle$, and the corresponding pointer state $|a_n\rangle$. This argument is based on the same idea of plausibility that characterize the qualitative description of the measuring process: in order to measure observables of \mathcal{S} when its state is $|s_n\rangle$ it is necessary that the measuring apparatus is driven in a correlated state $|a_n\rangle$ where the information about the state $|s_n\rangle$ is encoded.

In 1981 Zurek [90] first suggested that the preferred pointer basis is the one which preserves and contains information about the state of the system under measurement, that is the basis in which the system apparatus correlations $|s_n\rangle \otimes |a_n\rangle$ are left undisturbed by the subsequent formation of correlations with the environment. This idea can be translated in a sufficient criterion for dynamically stable pointer states: all pointer state projection operators P_n^A commute with the apparatus-environment interaction Hamiltonian $H_{\mathcal{A}\mathcal{E}}$:

$$[P_n^A, H_{\mathcal{A}\mathcal{E}}] = 0 \quad \forall n \quad (2.2)$$

The hypothesis is often referred to as “the environment performs a *non demolition measurement* of the apparatus”.

We indicate with $O_{\mathcal{A}}$ an observable for the apparatus \mathcal{A} . The formula (2.2) is satisfied if $H_{\mathcal{A}\mathcal{E}}$ is a function of $O_{\mathcal{A}}$, $H_{\mathcal{A}\mathcal{E}} = H_{\mathcal{A}\mathcal{E}}(O_{\mathcal{A}})$ so that the environment determines through the interaction $H_{\mathcal{A}\mathcal{E}}$, a preferred observable $O_{\mathcal{A}}$.

In our models the interaction mechanism is the diffusion process due to a scattering events of the particle (system \mathcal{S}) with an environment. The preferred pointer basis will be the one relative to the generalized eigenvectors of the position operator.

2.1.2 The local disappearance of the interference

In this section we analyze another general point of view about the environment, concerning the suppression of the interference terms in the reduced density matrix. Every possible observation on the system does not take into account the degrees of freedom of the environment.

Let us consider an observable $\hat{A}_{\mathcal{S}\mathcal{A}}$ for the subsystem $\mathcal{S} + \mathcal{A}$ and evaluate the expectation value:

$$\langle A_{\mathcal{S}\mathcal{A}} \rangle = \text{Tr}(\rho_{\mathcal{S}\mathcal{A}\mathcal{E}} [A_{\mathcal{S}\mathcal{A}} \otimes I_{\mathcal{E}}]) = \text{Tr}_{\mathcal{S}\mathcal{A}}(\rho_{\mathcal{S}\mathcal{A}} A_{\mathcal{S}\mathcal{A}}) \quad (2.3)$$

with

$$\rho_{\mathcal{S}\mathcal{A}\mathcal{E}} = \sum_{m,n} c_m c_n |s_m\rangle \otimes |a_m\rangle \otimes |e_m\rangle \langle s_n| \otimes \langle a_n| \otimes \langle e_n| \quad (2.4)$$

From the definition of partial trace:

$$\rho_{\mathcal{S}\mathcal{A}} = \text{Tr}_{\mathcal{E}}(\rho_{\mathcal{S}\mathcal{A}\mathcal{E}}) = \sum_{m,n} c_m c_n^* |s_m\rangle \otimes |a_m\rangle \langle s_n| \otimes \langle a_n| \quad (2.5)$$

The interference terms in $\rho_{\mathcal{S}\mathcal{A}}$, like $|s_m\rangle \otimes |a_m\rangle \langle s_n| \otimes \langle a_n|$ (with $m \neq n$), are a signature of the existence of quantum correlations between different *positions* of the pointer. In fact quantum interference effects for observables of macroscopic objects, as the positions of the pointer of \mathcal{A} , are never observed in practice. A conceivable explanation of the disappearance of the off-diagonal terms in (2.5) is based on the statement that different states of a macroscopic system, like the environment, are generically orthogonal. In fact it is enough that a microscopic subsystem of the environment is described by orthogonal states when $|e_m\rangle$ and $|e_n\rangle$ are the states characterizing the environment to make $|e_m\rangle$ and $|e_n\rangle$ orthogonal, even if they are macroscopically indistinguishable.

This point of view is generalized to conclude that the state of a subsystem of a macroscopic system is indistinguishable from a statistical sum as far as observables of the subsystem are concerned.

Bell [17] gave this point of view the name of FAPP (for all practical purposes) to stress the practical impossibility to observe quantum superpositions of the states of a macroscopic system.

In fact according to the FAPP hypothesis $\langle e_n | e_m \rangle \rightarrow \delta_{n,m}$ and the reduced density matrix becomes almost diagonal in the pointer basis $|a_n\rangle$:

$$\begin{aligned} \rho_{SA} &\longrightarrow \rho_{SA}^d \approx \sum_n |c_n|^2 |s_n\rangle \otimes |a_n\rangle \langle s_n| \otimes \langle a_n| \\ &= \sum_n |c_n|^2 P_n^S \otimes P_n^A \end{aligned} \tag{2.6}$$

in such a way that there is a suppression of the interference terms.

In the next chapter we will introduce specific models of quantum systems in interaction with some model environment where it is possible to analyze in some detail the dynamics of the suppression of the interference terms in the reduced density matrix of the system.

2.2 Models involving scattering

2.2.1 The Joos and Zeh model

The Joos and Zeh model is a *laboratory* for the study of the decoherence phenomenon induced by scattering processes. The first formulation dates back to 1985 and in the following years the model was generalized. One of the formulation of the model can be found in the work of Gallis and Fleming [45] that we will outline in this section.

Object of investigation is the asymptotic behavior of a *massive* particle surrounded by an environment composed by light particles.

Results are based on a fundamental assumption on the dynamic, originally formulated by Joos and Zeh. The hypothesis will be discussed in detail in the next section. Briefly it states that due to the very small ratio between the mass of the particles of the environment and the massive particle, there are two different time scales governing their dynamics: during the interaction the massive particle remains almost in the same place while the light ones are instantaneously projected in scattered states.

The hypothesis under the Joos and Zeh model are the following:

- the total system is isolated in a box with edge L
- spin is not included in the model
- there are many scattering events in the time unit
- the light particles are not interacting among each other.

With this assumptions it is possible to analyze the reduced density matrix, in the position representation, relative to the massive particle and to study the off-diagonal terms (the coherences). The damping or the disappearing of these last terms will be interpreted as a consequence of the interaction with the light particles. The position of the massive particle will be *more classical* because its state will show the structure of an incoherent superposition of “*eigenstates*” of the position operator.

The assumptions on the model listed above bring to the celebrated Joos and Zeh formula for the asymptotic behavior of the state of a massive and a light particle in interaction between them. The formula was never given a rigorous derivation either in the original work of Joos and Zeh or in the works of Gallis and Hornberger.

In the following chapter we give a rigorous and original derivation of the formula starting only from the dynamic of the interacting system.

In [53] the authors use the results they obtained to discuss the role of decoherence in the experimental setting for interference of matter waves with fullerene molecules engineered by the A.Zeilinger’s group in Wien.

2.2.2 Effect of a single scattering event

First of all in the Joos and Zeh model it has to be evaluated the effect of a single scattering event between a light particle and a massive particle.

According to the hypothesis of *recoilless* event, the state of the massive particle will be considered unperturbed by the scattering event. This conclusion is based on the following considerations.

The Schrödinger equation for a system composed of two different particles is:

$$H = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2m}\Delta_r + V(r - R) \quad (2.7)$$

where r is the position of the light particle, R in the position of the massive particle and $V(r - R)$ is the two body interaction potential while Δ_R and Δ_r represent the Laplace operators respectively on $L^2_R(\mathbb{R}^3)$ and $L^2_r(\mathbb{R}^3)$.

Performing a change of coordinates to the center of mass reference frame

$$\begin{aligned} L^2(\mathbb{R}^6, drdR) &\rightarrow L^2(\mathbb{R}^6, dx_1dx_2), \\ (Th)(x_1, x_2) &\equiv h \left(x_2 + \frac{M}{m+M}x_1, x_2 - \frac{m}{m+M}x_1 \right) \\ x_1 = r - R, \quad x_2 &= \frac{mr + MR}{m + M} \end{aligned} \quad (2.8)$$

where x_1 in the relative coordinate and x_2 is the position of the centre of mass, the equation (2.7) reads

$$THT^{-1} = H_0^\nu + H^\mu, \quad H_0^\nu = -\frac{\hbar^2}{2\nu}\Delta_{x_2}, \quad H^\mu = -\frac{\hbar^2}{2\mu}\Delta_{x_1} + V(x_1) \quad (2.9)$$

where μ is the reduced mass and ν is the total mass

$$\mu = \frac{mM}{m + M}, \quad \nu = m + M \quad (2.10)$$

Let $\epsilon = \frac{m}{M}$ be the mass ratio. In terms of ϵ we have

$$\begin{aligned} \mu &= \frac{\epsilon}{1 + \epsilon}M & \nu &= (1 + \epsilon)M \\ x_2 &= \frac{\epsilon r + R}{\epsilon + 1} \end{aligned} \quad (2.11)$$

In the new frame, posing $M = \hbar = 1$, the Schrödinger equation reads

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2(1 + \epsilon)}\Delta_{x_2}\psi - \frac{(1 + \epsilon)}{2\epsilon}\Delta_{x_1}\psi + V(x_1)\psi \quad (2.12)$$

Starting with a factorized initial condition $\psi(x_1, x_2) = \varphi(x_1)\phi(x_2)$ the dynamic of the two particles can be splitted as

$$i\frac{\partial\varphi}{\partial t} = -\frac{1}{2(1+\epsilon)}\Delta_{x_2}\varphi \quad (2.13)$$

$$i\frac{\partial\phi}{\partial t/\epsilon} = -\frac{(1+\epsilon)}{2}\Delta_{x_1}\phi + \epsilon V(x_1)\phi \quad (2.14)$$

The previous equations show explicitly that for a small mass ratio ϵ :

- the coordinate of the centre of mass is very similar to the position coordinate of the massive particle
- there are two dynamical regimes: *fast* motion of the light particle (2.14) described by a time parameter t/ϵ and a *slow* motion (2.13) of the massive one.

In this limit the interaction generates a fast diffusion process of the light particle from a scattering centre in a slow, almost free, motion.

In the work of Gallis and Fleming the following notation is used: $|\chi\rangle$ indicates the state of the light particle and $|R\rangle$ an "eigenstate" of the position operator for the massive particle at the initial time. The recoilless hypothesis for the massive particle and the accelerated dynamics for the light one is encoded into the following dynamical hypothesis, (**Joos e Zeh formula**)

$$(|R\rangle \otimes |\chi\rangle) \mapsto |x\rangle \otimes S^R(|\chi\rangle) \quad (2.15)$$

where S^R is the scattering operator relative to the interaction potential V centered in the R position (see [77]). The transition is supposed to happen in a very short time. For a more general initial condition, like a wave packet $\varphi(R)$, the Joos and Zeh formula becomes:

$$\int dR\varphi(R)|R\rangle|\chi\rangle \longrightarrow \int dR\varphi(R)|R\rangle S^R|\chi\rangle \quad (2.16)$$

The total density matrix after the interaction is

$$\rho = \int dRdR'\varphi(R)\varphi(R')|R\rangle\langle R'| \otimes S^R|\chi\rangle\langle\chi|(S^{R'})^\dagger \quad (2.17)$$

Tracing out over the degrees of freedom of the light particle we obtain the reduced density matrix describing the massive particle

$$\rho_S(R, R', t) = \rho_S(R, R', t_0)\langle\chi|(S^{R'})^\dagger, S^R|\chi\rangle \quad (2.18)$$

where $|\langle\chi|(S^{R'})^\dagger, S^R|\chi\rangle| \leq 1$ (the equal sign holding true only for $R = R'$) and t_0 and t are times shortly before and after the scattering process.

The last term shows explicitly the existence of a damping phenomenon for quantum correlations among distinct positions of the massive particle. In this sense the scattering event can be interpreted as the origin of the decoherence phenomenon.

2.2.3 Scattering with plane waves

For the analysis of (2.18) Gallis e Fleming have to assign a state for the environment particles. They used the eigenfunctions of the momentum operator. In the position representation $|y\rangle$ these eigenfunctions can be written as

$$\langle y|\chi\rangle \equiv \frac{1}{L^{\frac{3}{2}}} e^{\frac{i}{\hbar} p_A \cdot y} \quad (2.19)$$

The density matrix then reads

$$\rho_S(R, R', t) = \rho_S(x, x', t_0) \langle p_A | (S^{R'})^\dagger, S^R | p_A \rangle \quad (2.20)$$

where $|p_A\rangle$ is the vector state of the light particle with momentum p_A . The density matrix is evaluated using the relation

$$\langle p' | S_0 | p_A \rangle = \delta(p_A - p') + \frac{i}{2\pi\hbar|p_A|} f(p', p_A) \delta(|p_A| - |p'|) \quad (2.21)$$

where $f(p', p_A)$ is the scattering amplitude of V centered in the origin and S_0 is the corresponding scattering matrix.

The relation between S_0 and S^R is the following ([75]):

$$S^R = e^{-\frac{i}{\hbar} \hat{p} R} S_0 e^{-\frac{i}{\hbar} \hat{p} R} \quad (2.22)$$

Using the transition matrix T , formula (2.21) can be expressed as

$$\langle p' | T_0 | p_A \rangle = \frac{1}{2\pi\hbar|p_A|} f(p', p_A) \delta(|p_A| - |p'|) \quad (2.23)$$

The operator S is unitary:

$$S S^\dagger = \mathbb{I} \quad (2.24)$$

so that the operator T satisfies the following relation

$$i(T - T^\dagger) = -T T^\dagger \quad (2.25)$$

The time-reversal invariance of the scattering process implies

$$\langle p'' | T^\dagger T T | p' \rangle = \langle p' | T | p'' \rangle \quad (2.26)$$

where \mathcal{T} is the time inversion operator, from this we have that

$$\langle p' | T | p_A \rangle = \langle p_A | T | p' \rangle \quad (2.27)$$

The previous equality makes it possible to calculate $\langle p_A|(S^{R'})^\dagger, S^R|p_A\rangle$ as follows

$$\begin{aligned}
\langle p_A|(S^{R'})^\dagger, S^R|p_A\rangle &= \langle p_A|e^{-\frac{i}{\hbar}\hat{p}\cdot R'} S_0^\dagger e^{\frac{i}{\hbar}\hat{p}\cdot R'} e^{-\frac{i}{\hbar}\hat{p}\cdot R} S_0 e^{\frac{i}{\hbar}\hat{p}\cdot R}|p_A\rangle = \\
&= e^{-\frac{i}{\hbar}p_A R'} \langle p_A|S_0^\dagger e^{\frac{i}{\hbar}\hat{p}\cdot (R'-R)} S_0|p_A\rangle e^{\frac{i}{\hbar}p_A R'} = \\
&= e^{-\frac{i}{\hbar}p_A\cdot (R-R')} \sum_{p'} \left\{ e^{\frac{i}{\hbar}p_A\cdot (R-R')} [\langle p_A|p'\rangle \langle p'|p_A\rangle + \right. \\
&\quad \left. - \langle p_A|T_0|p'\rangle \langle p'|T_0^\dagger|p_A\rangle] + e^{\frac{i}{\hbar}p'\cdot (R'-R)} \langle p_A|T_0^\dagger|p'\rangle \langle p'|T_0|p_A\rangle \right\} = \\
&= 1 - \sum_{p'} |\langle p_A|T_0|p'\rangle|^2 \left(1 - e^{\frac{i}{\hbar}(p_A-p')(R-R')} \right) = \\
&= 1 - \sum_{p'} \frac{|f(p_A, p')|^2}{(2\pi)^2 \hbar p_A^2} \delta^2(|p_A| - |p'|) \left(1 - e^{\frac{i}{\hbar}(p_A-p')(R-R')} \right)
\end{aligned} \tag{2.28}$$

The assumptions about the state of the environmental light particles introduce into the model a formal problem, due to the presence of a $\delta^2(|p_A| - |p'|)$ in (2.28). In order to give sense to (2.28) Gallis and Fleming use the following procedure. They substitute into (2.28) the sum with the integral:

$$\sum_{p'} \rightarrow \left(\frac{2\pi\hbar}{L} \right)^3 \int d^3 p' \tag{2.29}$$

and one of the Dirac's δ is replaced with a discrete sum. Following this suggestion

$$\delta^2(p_A - p') = \frac{L}{\hbar} \delta(p_A - p') \tag{2.30}$$

from which

$$\begin{aligned}
\langle p_A|(S^{R'})^\dagger, S^R|p_A\rangle &= 1 - \frac{(2\pi)^3 \hbar}{L^3} \int d^3 p' \frac{1 - e^{\frac{i}{\hbar}(p_A-p')(R-R')}}{(2\pi)^2 p_A^2} |f(p_A, p')|^2 \delta^2(p_A - p') \\
&= 1 - \frac{(2\pi)}{L^2} \int d^3 p' \frac{1 - e^{\frac{i}{\hbar}(p_A-p')(R-R')}}{p_A^2} |f(p_A, p')|^2 \delta(p_A - p')
\end{aligned} \tag{2.31}$$

The generalization from a single event to a model of interaction with all the light particles of the environments requires an averaging over many events. One scattering event modifies the coherences in the reduced density matrix depending on the value of

$$\langle p_A|(S^{R'})^\dagger, S^R|p_A\rangle \tag{2.32}$$

If the value of this quantity is negligible the scattering event is defined as *effective*, if it assumes a unitary value it is defined as *ineffective*.

We can discuss what are the conditions for an ineffective event

$$\langle p_A | (S^{R'})^\dagger, S^R | p_A \rangle \approx 1 \quad \text{per } R \neq R' \quad (2.33)$$

This condition takes place when the incoming particle wave length λ_A satisfies

$$\lambda_A = \frac{\hbar}{p_A} \gg |R - R'| \quad (2.34)$$

or

$$\lambda_A = \frac{\hbar}{p_A} \ll |R - R'| \quad \text{and} \quad \sigma_{tot} \equiv \int d\Omega' |f(\hat{p}_A \cdot \hat{p}')|^2 \ll L^2 \quad (2.35)$$

We indicate with $\alpha \in [0, \pi]$ the angle between the vector $R - R'$ and $p_A - p'$

$$\frac{(R - R')(p_A - p')}{\hbar} = \frac{|R - R'| |p_A - p'|}{\hbar} \cos \alpha = \frac{|R - R'|}{\hbar} \sqrt{p_A^2 + p'^2 - 2p_A p' \cos \alpha} \quad (2.36)$$

we evaluate the previous formula for $p_A = p'$ and indicate with θ the angle between p_A and p'

$$\left. \frac{(R - R')(p_A - p')}{\hbar} \right|_{p_A=p'} = \frac{|R - R'| p_A}{\hbar} \sqrt{2 - 2 \cos \theta} \cos \alpha \quad (2.37)$$

If the condition $\frac{\hbar}{p_A} \gg |R - R'|$ holds the quantity (2.37) is negligible also for $|R - R'| \neq 0$; in this conditions the term $1 - e^{\frac{i}{\hbar}(R-R')(p_A-p')}$ appearing in (2.31) and the term $\langle p_A | (S^{R'})^\dagger, S^R | p_A \rangle$ tends to assume a unitary value.

When the wave length λ_A is much smaller than the length $|R - R'|$ the exponential term in (2.31) produces quick oscillations and the corresponding integral tends to be zero.

Indicating with Ω' the solid angle in \mathbb{R}^3 we have

$$\begin{aligned} \langle p_A | (S^{R'})^\dagger, S^R | p_A \rangle &= 1 - \frac{2\pi}{L^2} \int d^3 p' \frac{|f(p_A, p')|^2}{p_A^2} \delta(p_A - p') = \\ &= 1 - \frac{2\pi}{L^2} \int dp' \int d\Omega' p'^2 \frac{|f(p_A, p')|^2}{p_A^2} \delta(p_A - p') = \\ &= 1 - \frac{2\pi}{L^2} \int d\Omega' \left. \frac{|f(p_A, p')|^2}{p_A^2} \right|_{p_A=p'} = \\ &= 1 - \frac{2\pi}{L^2} \sigma_{tot} \end{aligned} \quad (2.38)$$

If $\sigma_{tot} \ll L^2$ the conditions of ineffective scattering event are true. For almost all models of physical environment that will be discussed in the rest of this

section the majority of the scattering events are to be considered ineffective. In spite of this the overall effect of decoherence will be proved to be relevant. This fact stresses that the decoherence phenomenon depends on the diffusion of quantum correlations toward the environment and not on the amount of energy exchanged.

The generalization to multiple scattering events requires two auxiliary hypothesis:

- let $\Delta t = t - t_0$ be the characteristic time interval of a macroscopic change in the system properties and τ the time interval between two scattering events. The first assumption reads

$$\tau \ll \Delta t \quad (2.39)$$

- the distribution of the momentum of the incoming particles is uniform and random

If these assumptions hold the scattering events are independent and random. According to (2.20) the change, during the time Δt of a single scattering event, in the reduced density matrix is

$$\rho_S(R, R', \Delta t) \left\{ \langle p_A | (S^{R'})^\dagger, S^R | p_A \rangle - 1 \right\} \quad (2.40)$$

The generalization to many scattering event reads

$$\Delta \rho_S(R, R', t = t_0 + \Delta t) = -\rho_S(R, R', t_0) \int \frac{d\Omega}{4\pi} \int dp \mathcal{N}^{\Delta t}(p) \left\{ 1 - \langle p | (S^{R'})^\dagger S^R | p \rangle \right\} \quad (2.41)$$

where $d\Omega$ is the solid angle singled out by the direction of p and $\mathcal{N}^{\Delta t}(p)$ is the number of particles, with impulse of modulo p , that in time Δt hit the surface L^2 . If $n(p)$ is the number of particles in the unitary volume with momentum p and velocity $v(p)$ the following relation holds

$$\mathcal{N}^{\Delta t}(p) = n(p) L^2 v(p) \Delta t \quad (2.42)$$

and

$$\frac{\Delta \rho_S(R, R', t)}{\Delta t} = -\rho_S(R, R', t_0) \int dp n(p) v(p) \int d\Omega d\Omega' \left. \frac{1 - e^{\frac{i}{\hbar}(p-p')(R-R')}}{2} \right|_{p=p'} |f(p, p')|^2 \quad (2.43)$$

When (2.39) holds

$$\frac{\partial \rho_S(R, R', t)}{\partial t} \approx \frac{\Delta \rho_S(R, R', t)}{\Delta t} \quad (2.44)$$

Defining the *localization function*

$$F(R - R') \equiv \int dp n(p) v(p) \int d\Omega d\Omega' \frac{1 - e^{\frac{i}{\hbar}(p-p')(R-R')}}{2} \Big|_{p=p'} |f(p, p')|^2 \quad (2.45)$$

it is possible to write the dynamical equation for ρ_S

$$\frac{\partial \rho_S(R, R', t)}{\partial t} \approx -\rho_S(R, R', t) F(R - R') \quad (2.46)$$

The previous equation has the following solution:

$$\rho_S(R, R', t) \approx \rho_S(R, R', t_0) e^{-F(R-R')(t-t_0)} \quad (2.47)$$

In order to give an easier expression of (2.45) the following expansion is used

$$1 - e^{\frac{i}{\hbar}(p-p')\Delta R} = 1 - \cos \frac{(p-p')\Delta R}{\hbar} - i \sin \frac{(p-p')\Delta R}{\hbar} \quad (2.48)$$

where $\Delta R = R - R'$.

The sine function is odd in the change of p and p' , while for the reciprocity theorem $|f(p, p')|$ is even so we will neglect the third term of (2.48) in the integral (2.45). The product between these terms is an odd function that gives a null contribution in (2.45)

The location function then reads

$$F(R - R') \equiv \int dp n(p) v(p) \int d\Omega d\Omega' \frac{1 - \cos \frac{i}{\hbar}(p-p')(R-R')}{2} \Big|_{p=p'} |f(p, p')|^2 \quad (2.49)$$

This function can be further analyzed. The argument of cosine in $F(R - R')$ is

$$\frac{1}{\hbar}(p-p')\Delta R = \frac{1}{\hbar}|p-p'|\Delta R \cos \alpha = \frac{|\Delta R|}{\hbar} \sqrt{p^2 + p'^2 - 2pp' \cos \alpha} \quad (2.50)$$

For $p = p'$ we have

$$\frac{1}{\hbar}(p-p')\Delta R \Big|_{p=p'} = \frac{|\Delta R|p}{\hbar} \sqrt{2 - 2 \cos \theta} \cos \alpha \quad (2.51)$$

For $|R - R'| \ll \lambda_A$ or $|\Delta R| \ll \frac{\hbar}{p}$ in (2.51) we get

$$\frac{1}{\hbar}(p-p')|\Delta R| \Big|_{p=p'} \ll 1 \quad (2.52)$$

Expanding the cosine function at the first order

$$1 - \cos \frac{(p - p')\Delta R}{\hbar} \Big|_{p=p'} \approx \frac{1}{2} \left(\frac{(p - p')\Delta R}{\hbar} \right)^2 \quad (2.53)$$

The location function can then be written as

$$F(R - R') \approx \frac{|R - R'|^2}{\hbar} \int_0^\infty dp p^2 n(p) v(p) 2\pi^2 \int_{-1}^1 d \cos \theta (1 - \cos \theta) |f(p, p')|^2 \quad (2.54)$$

Defining σ_{eff} as the effective cross section

$$\sigma_{eff} \equiv 2\pi^2 \int_{-1}^1 d \cos \theta (1 - \cos \theta) |f(p, p')|^2 \quad (2.55)$$

$$F(R - R') \approx |R - R'|^2 \Lambda \quad (2.56)$$

with

$$\Lambda = \int_0^\infty dp n(p) p^2 \frac{v(p) \sigma_{eff}}{\hbar^2} \quad (2.57)$$

the parameter Λ is defined as the location parameter and encode all the physical detail of the system under observation.

Typical values of Λ are reported in [57] and are reproduced in the following table where a is the radius of the massive particle

| | $a = 10^{-3}\text{cm}$ dust | $a = 10^{-5}\text{cm}$ dust | $a = 10^{-6}\text{cm}$ molecule |
|---|--------------------------------|--------------------------------|------------------------------------|
| Cosmic Ray Background | 10^6 | 10^{-6} | 10^{-12} |
| 300 K Photons | 10^{19} | 10^{12} | 10^6 |
| Sun ray (on the Earth) | 10^{21} | 10^{17} | 10^{13} |
| Air molecules | 10^{36} | 10^{32} | 10^{30} |
| Laboratory Void (10^3 particles/cm ³) | 10^{23} | 10^{19} | 10^{17} |

The location function can also be evaluated in a different approximation. Recall that for a single scattering event the dynamical evolution of the system \mathcal{S} can be described as

$$\rho_S(R, R', t) \equiv \rho_S(R, R', t_0) e^{-F(R - R')(t - t_0)} \quad (2.58)$$

with

$$F(R - R') = \int_0^\infty dp n(p) v(p) \int \frac{d\Omega d\Omega'}{2} \left(1 - \cos \frac{(p - p')(R - R')}{\hbar} \right) \Big|_{p=p'} |f(\hat{p} \cdot \hat{p}')|^2 \quad (2.59)$$

Consider now the case of a space separation such that

$$|R - R'| \gg \lambda_A \quad (2.60)$$

Recall that

$$\frac{(R - R')(p_A - p')}{\hbar} \Big|_{p_A=p'} = \frac{|R - R'| p_A}{\hbar} \sqrt{2 - 2 \cos \theta} \cos \alpha$$

We can perform the integration in $d\Omega'$

$$\begin{aligned} & \int d\Omega d\Omega' \cos \frac{(p - p')(R - R')}{\hbar} \Big|_{p=p'} |f(\hat{p}, \hat{p}')|^2 = \\ & = 4\pi \int d\Omega \cos \frac{p|R - R'|}{\hbar} \sqrt{2 - 2 \cos \theta} \cos \alpha |f(\hat{p}, \hat{p}')|^2 \end{aligned} \quad (2.61)$$

where $d\omega = \sin \theta d\theta d\phi$ and θ the angle between p and p' .

If $|f(\hat{p}, \hat{p}')|^2$ is sufficiently regular and $|R - R'|p/\hbar$ is large (in the sense of the previous approximation) the integral does not influence the location function. Then

$$F(R - R') \simeq \int_0^\infty dp n(p) v(p) \int \frac{d\Omega d\Omega'}{2} |f(\hat{p}, \hat{p}')|^2 \quad (2.62)$$

recalling the definition of cross section and performing the integration in $d\Omega'$ finally we obtain

$$\begin{aligned} F(R - R') & \simeq \int_0^\infty dp n(p) v(p) \int \frac{d\Omega d\Omega'}{2} |f(\hat{p}, \hat{p}')|^2 \\ & = 2\pi \int_0^\infty dp n(p) v(p) \sigma_{tot}(p) \equiv F(\infty) = cost. \end{aligned} \quad (2.63)$$

2.3 A more realistic model

2.3.1 Massive particle interacting with a thermal bath

In this section we consider a somehow more realistic formulation of the Joos and Zeh model elaborated by K.Hornberger and J.E.Sipe ([52]). In this work the authors analyze the decoherence effects on a massive particle induced by the collisions between with a thermal bath. The particles of the environment are represented as wave packets. In this way the formal contradictions seen before are not present.

K.Hornberger and J.E.Sipe first noticed that the evolution process from the interaction time to $t = \infty$ is in general not described by the scattering operator S as it appears in the Joos and Zeh formula. The scattering process S describes the evolution from a remote past time to a faraway future. The authors suggest a change in the formula that we discuss in the chapter 4.

In the following we want summarize some results given in [52].

The environment is described as a thermal bath with equilibrium temperature $k_B T = \beta^{-1}$. The density matrix for every light particle is

$$\rho^{bath} = \frac{\lambda^3}{\Omega} e^{-\beta p^2/2m} \quad (2.64)$$

where Ω is the volume, m is the mass of a light particle and λ the de Broglie wave length.

$$\lambda = \sqrt{\frac{2\pi\hbar^2\beta}{m}} \quad (2.65)$$

The estimate of the scattering effect due to the thermal bath requires the following assumptions:

- the bath particle density is small compared with λ^{-3} . With this assumption the bath state is a product of single particle states
- the characteristic time of observation Δt is long enough to allow a wave packet displacement larger than its amplitude and than the distance from two scattering points.

Based on this hypothesis the authors obtain the evolution equation

$$\frac{\partial}{\partial t} \rho(R, R') = -F(R - R') \rho(R, R'; t) \quad (2.66)$$

where

$$F(R) = n \int_0^\infty dq \nu(q) \frac{q}{m} \int \frac{d\hat{n}_1 d\hat{n}_2}{4\pi} (1 - e^{iq(\hat{n}_1 - \hat{n}_2)R/\hbar}) |f(q\hat{n}_2, q\hat{n}_1)|^2$$

$\nu(q)$ is the momentum Maxwell distribution, $d\hat{n}_i$ indicates integration over the sphere of unitary radius and n is the bath particle density.

Both models finally obtain a similar evolution in the form

$$\rho_S(R, R', t) \approx \rho_S(R, R', t_0) e^{-F(R-R')(t-t_0)} \quad (2.67)$$

where the decoherence function F is defined as

$$F(R - R') \approx \begin{cases} \Lambda |R - R'| & \text{if } |R - R'| \ll \lambda_A \\ \epsilon n \int dq \nu(q) \sigma(q) & \text{if } |R - R'| \gg \lambda_A \end{cases} \quad (2.68)$$

In Hornberger and Sipe work ϵ takes value 1 while in the original Joos and Zeh model it assumes the value 2π .

The successive work of Hornberger and Sipe [52] tends to support the result that the right choice of the value of ϵ is 1.

Chapter 3

Point Interaction

In the previous chapter we analyzed a particular model of quantum environment acting on the system under consideration by frequent scattering events. Only the single event was analyzed according to quantum theory whereas the collective effect of the environment was deduced by an essentially statistical reasoning.

In the following chapter we describe a constructive approach to the modeling of a quantum environment. The dynamics we want to analyze is the one given by the Schrödinger equation for the entire system without any statistical assumption. Of course this choice forces to analyze only oversimplified systems showing a very simple dynamical behavior. The main technical tool in our models is presented in this chapter.

3.1 Brief history of point interaction

In this section we sketch a short history of point interactions.

The first relevant model in quantum mechanics based on point interactions has been elaborated by Kronig and Penney [63] in 1931 in order to analyze the dynamics of electrons in solids. These authors considered a one dimensional model for the motion of an electron in a periodic potential: the ions are fixed and placed on the sites of a regular one dimensional lattice. Every ion is supposed to act on each electron in the conduction band via a zero range potential. The electrons are considered non interacting among themselves. The Hamiltonian for one electron in the conduction band is written formally as

$$H^{KP} = -\frac{d^2}{dx^2} + \sum_j \alpha_j \delta_{y_j} \quad (3.1)$$

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 one dimension $-\Delta + \sum_j \alpha_j \delta_{y_j}$ corresponds to the Laplacian acting on functions which are continuous with first derivative discontinuous in y_j and satisfying boundary conditions

$$\psi'(y_j^+) - \psi'(y_j^-) = \alpha_j \psi(y_j) \quad \forall j. \quad (3.2)$$

Using these boundary conditions Kronig and Penney studied the spectral properties of the Hamiltonian (3.1). They found a non trivial band structure whose parameters were explicitly computable. After 80 years Kronig and Penney model remains one of the few periodic potential Hamiltonian completely solvable in quantum mechanics.

In 1935 the study of Hamiltonians with zero range potential in dimension three started. In that year Bethe and Peierls [21] published a work about a two body system with a zero range attractive potential: this system is a model for the deuteron, a physical system characterized by a strong interaction between a proton and a neutron. Using point interaction for the first time in nuclear physics Bethe and Peierls produced a solvable model of the deuteron photodisintegration.

In the same year Thomas [85] started the study of zero range Hamiltonians (3.1) in dimension three obtaining them as limit of local, rescaled short-range potentials. He first noticed that a renormalization of the coupling constant was necessary.

In 1936 Fermi [42] obtained the same results in his work about the motion of neutrons in hydrogenous substances. Fermi described the interaction between the proton and the neutron with a delta potential. For this reason, especially in nuclear physics, point interactions are referred to as Fermi pseudo-potentials. In 1961 Berezin and Faddeev [19] gave the first precise mathematical definition of Hamiltonians like (3.1) in dimension three. For the first time the Hamiltonian was written as a self-adjoint operator derived by Krein's theory of self-adjoint extensions of symmetric operators.

Nowadays the entire class of point interaction Hamiltonians is completely characterized. The reader can refer to [9] for the details of the theory and for a complete list of references.

There are two different approaches to the definition of selfadjoint operators describing point interactions: the first one is based on the well known von Neumann formula, the second one uses a relation called Krein formula. Results are equivalent but while the first approach allows an immediate definition of the domain of these operators, the second one makes immediately available their spectral properties. In the last years K.Pankrashkin and S.Albeverio [68], [11] gave an alternative procedure of construction of point interactions based on generalized boundary conditions. This last approach is presented in Appendix B.

The connection between the various approaches to the theory of self-adjoint extensions is clearly explained in a recent work of A.Posilicano [72]. Examples

of recent applications of point interaction Hamiltonians in modern mathematical physics concerning time dependent and non-linear problems are contained in [32], [33], [1], [3], [2].

3.2 Singular Perturbations of the Laplacian

In this section we discuss the selfadjoint realizations of the formal expression (3.1). Intuitively a point interaction Hamiltonian should act as the free laplacian on functions which are zero in the vicinities of the interaction centers. This suggests the following procedure: if $\{y_1, \dots, y_n\}$ with $y_i \in \mathbb{R}^d$ is the set of interaction centers, let us define $C_0^\infty(\mathbb{R}^d \setminus \{y_1, \dots, y_n\})$ to be the set of functions which are differentiable infinitely many times and whose support does not contain any interaction center.

Let us define the following operator

$$\hat{H} = -\Delta, \quad D(\hat{H}) = C_0^\infty(\mathbb{R}^d \setminus \{y_1, \dots, y_n\}) \quad (3.3)$$

All the non-trivial extensions of \hat{H} (if any) will be given the name of Hamiltonian with point interactions placed in the points y_i . In fact operator (3.3) is symmetric but not selfadjoint in $L^2(\mathbb{R}^d)$; one selfadjoint extension of (3.3) is trivial, i.e. the free laplacian $H_0 = -\Delta$.

Let us start the characterization of the domain of \hat{H}^* adjoint to \hat{H} . In the following we will indicate with $H^2(\mathbb{R}^d)$ the standard Sobolev space of functions in $L^2(\mathbb{R}^d)$ together with their first and second derivative, with norm

$$\|\psi\|_{H^2} = \int (1 + |k|^2)^2 |\tilde{\psi}(k)| dk$$

For any function $\psi \in H^2(\mathbb{R}^d)$ and $\phi \in D(\hat{H})$, we have

$$(\psi, -\Delta\phi) = (-\Delta\psi, \phi)$$

where (\cdot, \cdot) is the inner product in $L^2(\mathbb{R}^d)$.

Any function in $H^2(\mathbb{R}^d)$ then belongs to the domain of the operator \hat{H}^* because

$$|(\psi, -\Delta\psi)| \leq \|\psi\|_{H^2} \|\psi\|_{L^2}$$

It is also true that

$$(G_i^z, \hat{H}\phi) = (zG_i^z, \phi) \quad \phi \in D(\hat{H}) \quad i = 1, \dots, n \quad z \in \mathbb{C} \setminus \mathbb{R} \quad (3.4)$$

where G_i^z denotes the inverse Fourier transform of

$$\tilde{G}_i^z = \frac{e^{ik \cdot y_i}}{k^2 - z} \quad (3.5)$$

In fact the G_i^z and their derivatives are the only solutions of $(-\Delta + z)\phi = 0$ outside y_i . This means that the eigenspaces $\mathcal{N}^z \in L^2(\mathbb{R}^d)$ of the adjoint \hat{H}^* of \hat{H} relative to the eigenvalue z is generated by all the G_i^z and their derivatives as long as they belong to $L^2(\mathbb{R}^d)$.

The behavior at infinity of the G_i^z imply

- for $d = 1$ the G_i^z and their first derivatives belong to $L^2(\mathbb{R})$;
- for $d = 2, 3$ the G_i^z belong to $L^2(\mathbb{R}^d)$ but their derivatives do not;
- for $d > 3$ no function in $L^2(\mathbb{R}^d)$ satisfies (3.4).

It is possible to show (see e.g. Theorem X.1 in [76]) that the dimension of \mathcal{N}^z is constant as z varies over the complex plane, outside the positive real axis. Conventionally \mathcal{N}^i and \mathcal{N}^{-i} play a special role and are referred to as *deficiency subspaces*. The numbers $n_+ = \dim[\mathcal{N}^i]$ and $n_- = \dim[\mathcal{N}^{-i}]$ are called *deficiency indices*; they are non negative integers possibly equal to infinity.

$D(\hat{H}^*)$ can be written in an alternative way: first of all note that $G_i^{z_1} - G_i^{z_2}$ for $z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}^+$ belongs to $H^2(\mathbb{R}^d)$

$$(-\Delta - z_1)G_i^{z_1} - (-\Delta - z_2)G_i^{z_2} = 0 \implies \Delta(G_i^{z_1} - G_i^{z_2}) = -z_1G_i^{z_1} + z_2G_i^{z_2} \in L^2(\mathbb{R}^d)$$

The linear combinations $f + g$ of functions $f \in H^2(\mathbb{R}^d)$ and $g \in \mathcal{N}^{\hat{z}}$, for some \hat{z} , exhaust all linear combinations of the same kind with $g \in \mathcal{N}^z$ for any $z \in \mathbb{C} \setminus \mathbb{R}^+$. It is not hard to prove that it is possible to express any function in $D(\hat{H}^*)$ as a linear combinations of a function in $H^2(\mathbb{R}^d)$ and a function in $\mathcal{N}^{\hat{z}}$ for some $\hat{z} \in \mathbb{C} \setminus \mathbb{R}^+$.

The functions in $D(\hat{H}^*)$ can be chosen as a linear combination of $f \in H^2(\mathbb{R}^d)$, such that $f(y_i) = 0$ for $i = 1, 2, \dots, n$, and functions in \mathcal{N}^{z_1} and \mathcal{N}^{z_2} , with fixed $z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}^+$. In fact the regular part of $\alpha G_i^{z_1} + \beta G_i^{z_2}$ in y_i can assume an arbitrary value.

This result can be viewed as an application of a general result known as the Von Newman formula stating that: if A is a densely defined closed symmetric operator on a separable Hilbert space and A^* its adjoint then for all $z \in \mathbb{C} \setminus \mathbb{R}$

$$D(A^*) = D(A) \oplus \mathcal{N}^z(A) \oplus \mathcal{N}^{\bar{z}}(A). \quad (3.6)$$

It is not hard to convince oneself that A is self-adjoint if and only if $n_+(A) = n_-(A) = 0$, in fact, in this case, A is symmetric and $D(A) = D(A^*)$.

If $n_+ = n_- > 0$ formula (3.6) suggests the strategy to find the self-adjoint extensions of A_0 . In fact from (3.6) if $\psi \in D(A^*)$

$$\psi = \psi_0 + \phi^z + \phi^{\bar{z}} \quad \psi_0 \in D(A), \phi^z \in \mathcal{N}^z, \phi^{\bar{z}} \in \mathcal{N}^{\bar{z}} \quad (3.7)$$

and

$$A^*\psi = A\psi_0 + z\phi^z + \bar{z}\phi^{\bar{z}}. \quad (3.8)$$

If \hat{A} is an extension of A the following chain of inclusions holds

$$A \subseteq \hat{A} \subseteq \hat{A}^* \subseteq A^* \quad (3.9)$$

and $D(\hat{A}^*)$ must be obtained by $D(A^*)$ restricting the subspace $\mathcal{N}^z \oplus \mathcal{N}^{\bar{z}}$.

Suppose that $(\phi^z + \phi^{\bar{z}}) \in D(\hat{A}^*)$, by straightforward calculations one can check that

$$\left(\phi^z + \phi^{\bar{z}}, \hat{A}^*(\phi^z + \phi^{\bar{z}}) \right) - \left(\hat{A}^*(\phi^z + \phi^{\bar{z}}), \phi^z + \phi^{\bar{z}} \right) = (z - \bar{z}) (\|\phi^z\|^2 - \|\phi^{\bar{z}}\|^2) \quad (3.10)$$

Then \hat{A}^* is symmetric if and only if $\phi^{\bar{z}} = U\phi^z$ with U an isometric application from \mathcal{N}^z to $\mathcal{N}^{\bar{z}}$. If $\dim(\mathcal{N}^z) = \dim(\mathcal{N}^{\bar{z}})$ then the application U is unitary. In this case domain and action of A^U by (3.7) and (3.8) are

$$D(A^U) = \{\psi = \psi_0 + \phi^z + U\phi^z : \psi_0 \in D(A), \phi^z \in \mathcal{N}^z(A)\} \quad (3.11)$$

$$A^U(\psi_0 + \phi^z + U\phi^z) = A\psi_0 + z\phi^z + \bar{z}U\phi^z \quad (3.12)$$

and the operator is self-adjoint.

Such construction does not work if $n_+ \neq n_-$, then self-adjoint extensions of a symmetric operator A exist if and only if $n_+(A_0) = n_-(A_0) > 0$ and every self-adjoint extension of A is an element of a family of self-adjoint operators parameterized by unitary applications U between $\mathcal{N}^z(A)$ and $\mathcal{N}^{\bar{z}}(A)$. Given U , the corresponding self-adjoint operator A^U is defined by (3.11) and (3.12).

The Krein's formula for the resolvent gives different and sometimes easier characterization of self-adjoint extensions and a more direct way in order to obtain their spectral properties.

Assume that A 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 then an operator \ddot{A} exists such that $\ddot{A} \subseteq A^U$, $\ddot{A} \subseteq A^V$ and \ddot{A} extends any operator B that fulfills $B \subseteq A^U$, $B \subseteq A^V$, \ddot{A} is called the maximal common part of A^U and A^V . The deficiency indices of \ddot{A} are (m, m) with $0 < m \leq n$. A set $\{\phi_1^z, \dots, \phi_m^z\}$ of independent solutions of

$$\ddot{A}^*\phi^z = z\phi^z \quad \phi^z \in D(\ddot{A}^*), \quad z \in \mathbb{C} \setminus \mathbb{R} \quad (3.13)$$

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

$$(A^U - z)^{-1} - (A^V - z)^{-1} = \sum_{i,j=1}^m \Gamma(z)_{ij}^{-1} (\phi_j^{\bar{z}}, \cdot) \phi_i^z \quad z \in \rho(A^U) \cap \rho(A^V) \quad (3.14)$$

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

$$\Gamma(z)^* = \Gamma(\bar{z}) \quad z \in \rho(A^U) \cap \rho(A^V) \quad (3.15)$$

where $*$ indicates the Hermitian conjugate. Functions $\Gamma(z)_{ij}$ and ϕ_i^z , $i, j = 1, \dots, m$, may be chosen to be analytic for $z \in \rho(A^U) \cap \rho(A^V)$. In fact ϕ_i^z may be defined as

$$\phi_i^z = \phi_i^{z_0} + (z - z_0)(A^V - z)^{-1}\phi_i^{z_0} \quad i = 1, \dots, m, \quad z \in \rho(A^V) \quad (3.16)$$

where $\phi_i^{z_0}$, $i = 1, \dots, m$, $z_0 \in \mathbb{C} \setminus \mathbb{R}$, are linearly independent solutions of equation (3.13) with $z = z_0$ and matrix $\Gamma(z)$ as

$$\begin{aligned} \Gamma(z)_{ij} = \Gamma(z')_{ij} - (z - z')(\phi_j^{\bar{z}}, \phi_i^{z'}) \quad & i, j = 1, \dots, m \\ z, z' \in \rho(A^U) \cap \rho(A^V) \end{aligned} \quad (3.17)$$

where ϕ_i^z , $i = 1, \dots, m$ are defined according to (3.16).

The strategy in order to obtain a selfadjoint extension of a symmetric operator using the Krein's formula is the following: starting with a symmetric operator A we choose a selfadjoint extension A_0 , and the maximal common part between A and A_0 . All the selfadjoint extensions are then fixed by the Krein formula and by the resolvent of A_0 .

The Krein formula mentioned before in this chapter is not the most general relation between resolvents of two selfadjoint extensions of the same operator. The most general form is described in Appendix B

3.2.1 Point interaction in \mathbb{R}^3

In this section we first apply both the above discussed procedures in order to obtain self adjoint operators describing point interaction in \mathbb{R}^3 with only one point placed in $y \in \mathbb{R}^3$. At the end of this section we summarize the results for n points in \mathbb{R}^3 .

The Green's function G_i^z in \mathbb{R}^3 reads

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

where we have omitted the dependence from the point. From (3.6) and (3.7) we have the following description of the domain of the adjoint of \hat{H} :

$$D(\hat{H}^*) = \{f \in L^2(\mathbb{R}^3) | f = f_0 + \beta G^z(\cdot - y) + \gamma G^{\bar{z}}(\cdot - y)\}$$

where $f_0 \in H^2(\mathbb{R}^3 \setminus \{y\})$ and

$$\hat{H}^* f = -\Delta f_0 + \beta z G^z(\cdot - y) + \gamma \bar{z} G^z(\cdot - y)$$

A direct computation gives

$$\begin{aligned} & \left([\beta G^z(\cdot - y) + \gamma G^z(\cdot - y), \hat{H}^* [\beta G^z(\cdot - y) + \gamma G^z(\cdot - y)]] \right) = \\ & = (|\beta|^2 z + |\gamma|^2 \bar{z}) \|G^z\| + 2\Re(\bar{\gamma}\beta(G^{\bar{z}}, G^z)) \end{aligned}$$

showing that \hat{H}^* acts as a symmetric operator on linear combinations of G^z and $G^{\bar{z}}$ if and only if $\|\beta\| = \|\gamma\|$. There are then infinitely many selfadjoint extension of \hat{H} (equivalently selfadjoint restrictions of \hat{H}^*) defined in the following way

$$D(H_{\phi,y}^{3d}) = \{f \in L^2(\mathbb{R}^3) | f = f_0 + \beta G^z(\cdot - y) + \beta e^{i\phi} G^{\bar{z}}(\cdot - y)\}$$

$$H_{\phi,y}^{3d} f = -\Delta f_0 + \beta z G^z + \beta e^{i\phi} \bar{z} G^{\bar{z}} \quad (3.18)$$

An alternative description of the family of selfadjoint extensions $H_{\phi,y}^{3d}$ is obtained in the following way: take λ positive large enough and define $G_\lambda = G^{z=-\lambda}$. Notice that, around $x = y$

$$\begin{aligned} & G^z(x - y) + e^{i\phi} G^{\bar{z}}(x - y) - (1 + e^{i\phi}) G_\lambda(x - y) = \\ & = \frac{i\sqrt{z}}{4\pi} + e^{i\phi} \frac{i\sqrt{\bar{z}}}{4\pi} + \frac{\sqrt{\lambda}}{4\pi} (1 + e^{i\phi}) + f_0 \\ & = (1 + e^{i\phi}) \left(\alpha + \frac{\lambda}{4\pi} \right) + f_0 \end{aligned} \quad (3.19)$$

where f_0 is a regular function taking value zero in $x = y$ and

$$\alpha = \frac{\Re\sqrt{z}}{4\pi} \tan \frac{\phi}{2} - \frac{\Im\sqrt{z}}{4\pi}$$

Formula (3.84) allows to characterize functions in the domains of the different selfadjoint extensions as a relation connecting the behaviour of the functions at the singularity ($\beta(1 + e^{i\phi})/4\pi|x - y|$ in our case) and the value taken at the same point by their regular part. More precisely for any $\alpha \in \mathbb{R}$ there is a selfadjoint extension of \hat{H} defined in the following way

$$D(H_{\alpha,y}^{3d}) = \left\{ f \in L^2(\mathbb{R}^3) | f = \Phi_\lambda + q^{3d} G_\lambda(\cdot - y) \quad \Phi_\lambda \in H^2(\mathbb{R}^3) \quad q = \frac{\Phi_\lambda(y)}{\alpha + \sqrt{\lambda}/4\pi} \right\} \quad (3.20)$$

Taking into account that $G^z(x-y) + e^{i\phi}G^{\bar{z}}(x-y) - (1 + e^{i\phi})G_\lambda(x-y) \in H^2(\mathbb{R}^3)$ and that

$$\begin{aligned} -\Delta (G^z(x-y) + e^{i\phi}G^{\bar{z}}(x-y) - (1 + e^{i\phi})G_\lambda(x-y)) = \\ = zG^z(x-y) + e^{i\phi}\bar{z}G^{\bar{z}}(x-y) + (1 + e^{i\phi})\lambda G_\lambda(x-y) \end{aligned}$$

the action of $H_{\alpha,y}^{3d}$ on $D(H_{\alpha,y}^{3d})$ is easily found to be

$$(H_{\alpha,y}^{3d} + \lambda)f = (-\Delta + \lambda)\Phi_\lambda \quad (3.21)$$

The expression (3.20) implies that the action of $(H_{\alpha,y}^{3d} + \lambda)^{-1}$ does not differ from the action of $(-\Delta + \lambda)^{-1}$ on functions of $H^2(\mathbb{R}^3 \setminus \{y\})$ (being $q = 0$ in this case). On the other hand

$$((H_{\alpha,y}^{3d} + \lambda)^{-1} - (-\Delta + \lambda)^{-1})G_\lambda, (\hat{H} + \lambda)g = 0$$

for any g in the set $C_0^\infty(\mathbb{R}^3 \setminus \{y\})$ which is dense in $L^2(\mathbb{R}^3)$. As a consequence the function $(H_{\alpha,y}^{3d} + \lambda)^{-1} - (-\Delta + \lambda)^{-1})G_\lambda$ belongs to $\mathcal{N}_{-\lambda}$ which in turn means that it is proportional to G_λ itself. The two resolvents then differ on the one dimensional subspace generated by G_λ . Being $D(H_{\alpha,y}^{3d})$ in (3.20) the range of $(H_{\alpha,y}^{3d} + \lambda)^{-1}$ one finally obtains

$$[(H_{\alpha,y}^{3d} + \lambda)^{-1}f](x) = (G_\lambda g)(x) + \frac{1}{\alpha + \sqrt{\lambda}/4\pi} G_\lambda(x-y)(G_\lambda g)(y) \quad (3.22)$$

The same expression of (3.22) can be easily obtained from the Krein formula (3.14). Note that the function

$$\Gamma(z) = -i\frac{\sqrt{z}}{4\pi} + \alpha \quad (3.23)$$

where α is a real constant, satisfies

$$\Gamma(z) - \Gamma(z') = (z' - z)(G^{\bar{z}}, G^{z'}) \quad z, z' \in \rho(H_{\alpha,y}^{3d}) \quad (3.24)$$

where with $\rho(H_{\alpha,y}^{3d})$ we have indicated the resolvent set for $H_{\alpha,y}$ and

$$\overline{\Gamma(z)} = \Gamma(\bar{z}) \quad (3.25)$$

From Krein's formula one obtains

$$(H_{\alpha,y}^{3d} - z)^{-1} = (H_0 - z)^{-1} + \frac{4\pi}{4\pi\alpha - i\sqrt{z}} (G^{\bar{z}}(\cdot - y), \cdot) G^z(\cdot - y) \quad (3.26)$$

From the explicit expression of the resolvent (3.22) one can easily deduce the spectral properties $H_{\alpha,y}$

- the spectrum of $H_{\alpha,y}^{3d}$ is

$$\sigma(H_{\alpha,y}^{3d}) = [0, \infty) \quad \alpha \geq 0$$

$$\sigma(H_{\alpha,y}^{3d}) = \{-16\pi^2\alpha^2\} \cup [0, \infty) \quad \alpha < 0$$

- for $\alpha < 0$ the only eigenvalue is simple and the corresponding normalized eigenfunction is

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

- for any $\alpha \in \mathbb{R}$, corresponding to each positive energy E in the continuous spectrum there are infinitely many generalized eigenfunction

$$\Phi_{\alpha,y,\pm}^{3d}(x, k) = e^{ikx} + \frac{e^{iky}}{4\pi\alpha \pm i|k|} \frac{e^{\mp i|k||x-y|}}{|x-y|} \quad (3.27)$$

with $|k|^2 = E$.

Using the generalized eigenfunctions $\Phi_{\alpha,y,\pm}^{3d}$ it is possible to define the unitary maps (see e.g. [40]) $\mathcal{F}_\pm^y : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$

$$[\mathcal{F}_\pm^y f](k) = s - \lim_{R \rightarrow \infty} \frac{1}{(2\pi)^{3/2}} \int_{B_R} \overline{\Phi_{\alpha,y,\pm}^{3d}(x, k)} f(x) dx \quad (3.28)$$

where B_R indicates the sphere of radius R in \mathbb{R}^3 . The wave operators (see e.g. [77] and [83]) for the Hamiltonian $H_{\alpha,y}^{3d}$

$$\Omega_\pm^y = s - \lim_{\tau \rightarrow \pm\infty} e^{i\tau H_{\alpha,y}^{3d}} e^{-i\tau H_0} \quad (3.29)$$

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

$$\Omega_\pm^y = (\mathcal{F}_\pm^y)^{-1} \mathcal{F} ; \quad (\Omega_\pm^y)^{-1} = \mathcal{F}^{-1} \mathcal{F}_\pm^y \quad (3.30)$$

where \mathcal{F} indicates the usual Fourier transform.

The explicit form of the spectral decomposition of $H_{\alpha,y}^{3d}$ in terms of the eigenfunctions allows us to write the solution of the Schrödinger equation

$$i \frac{\partial \psi_t}{\partial t} = H_{\alpha,y} \psi_t \quad (3.31)$$

corresponding to any initial state in $L^2(\mathbb{R}^3)$ as an integral over the spectral measure. In fact the integral kernel, in configuration space, for the propagator

of $H_{\alpha,y}^{3d}$ can be explicitly computed ([79], [10])

$$\begin{aligned}
U_{\alpha}^t(x, x') &= U^t(x - x') + \frac{2it}{|x - y||x' - y|} U^t(|x - y| + |x' - y|) + \\
&+ \begin{cases} -\frac{8\pi\alpha it}{|x - y||x' - y|} \int_0^{\infty} e^{-4\pi\alpha u} U^t(u + |x - y| + |x' - y|) du & \alpha > 0 \\ 0 & \alpha = 0 \\ 2|\alpha| e^{4\pi i|\alpha|^2 t} \frac{e^{-4\pi|\alpha||x-y|}}{|x-y|} \frac{e^{-4\pi|\alpha||x'-y|}}{|x'-y|} + \\ + \frac{8\pi\alpha it}{|x - y||x' - y|} \int_0^{\infty} e^{4\pi\alpha u} U^t(u - |x - y| - |x' - y|) du & \alpha < 0 \end{cases} \quad (3.32)
\end{aligned}$$

where $U^t(x - x')$ is the integral kernel of the “free” propagator $e^{-iH_0 t}$ in dimension three

$$(e^{-iH_0 t} f)(x) = \int_{\mathbb{R}^3} U^t(x - x') f(x') dx' = \int_{\mathbb{R}^3} \frac{e^{i\frac{|x-x'|^2}{4t}}}{(4\pi it)^{\frac{3}{2}}} f(x') dx' \quad (3.33)$$

A formal Laplace transform of (3.22) suggests for the solution of the Schrödinger equation (3.31) the following formula, showing a free-propagation contribution and a term representing spherical waves generated at the interaction center

$$\psi_t(x) = (U(t)\psi_0)(x) + i \int_0^t ds U(t - s, |x - y|) q(s) \quad (3.34)$$

where $U(t)$ is the propagator of the free unitary group defined by the kernel

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

One find easily that (3.34) is the solution of the Schrödinger equation (3.31) corresponding to an initial condition $\psi_0 \in D(H_{\alpha,y}^{3d})$ if the function $q(t)$ satisfies the Volterra integral equation

$$q(t) + 4\sqrt{i\pi}\alpha \int_0^t ds \frac{q(s)}{\sqrt{t-s}} = 4\sqrt{i\pi} \int_0^t ds \frac{(U(s)\psi_0)(y)}{\sqrt{t-s}} \quad (3.35)$$

More precisely one can prove that if $q(t)$ is the unique solution of (3.35) then (3.34) defines a function ψ_t which for any $t \geq 0$ belongs to $D(H_{\alpha,y}^{3d})$ ($q(t)$ being the coefficient of the singular part of ψ_t) and satisfies (3.31). Notice that Schrödinger dynamics is explicitly known if one can solve the Volterra integral equation (3.35).

Now we want to summarize the results for the most general case of n point interactions placed in $Y = \{y_1, \dots, y_n\}$, $y_i \in \mathbb{R}^3$ with parameters of interaction $\alpha = \{\alpha_1, \dots, \alpha_n\}$.

Without going into the details of the construction (for a complete description see [86], [9]) we simply recall the properties of the so called local point interactions, characterized by generalized boundary conditions in each y_i , $i = 1, \dots, n$. The domain and the action are:

$$D(H_{\alpha,Y}^{3d}) = \left\{ u \in L^2(\mathbb{R}^3) \mid u = \phi^\lambda + \sum_{k=1}^n q_k G_\lambda(\cdot - y_k), \right. \quad (3.36)$$

$$\left. \phi^\lambda \in H^2(\mathbb{R}^3), \phi^\lambda(y_j) = \sum_{k=1}^n [\Gamma_{\alpha,y}^{3d}(\lambda)]_{jk} q_k, j = 1, \dots, n \right\} \quad (3.37)$$

$$(H_{\alpha,Y}^{3d} + \lambda)u = (-\Delta + \lambda)(u - G_Y^\lambda q) \quad (3.38)$$

where

$$[\Gamma_{\alpha,Y}^{3d}(\lambda)]_{jk} = \left(\alpha_j + \frac{\sqrt{\lambda}}{4\pi} \right) \delta_{jk} - G^\lambda(y_j - y_k)(1 - \delta_{jk}) \quad (3.39)$$

At each point y_j the elements of the domain satisfy a boundary condition expressed by the last equality in (3.37). If we define $r_j = |x - y_j|$ it is easy to see that the boundary conditions can be equivalently written

$$\lim_{r_j \rightarrow 0} \left[\frac{\partial(r_j u)}{\partial r_j} - 4\pi \alpha_j(r_j u) \right] = 0, \quad j = 1, \dots, n \quad (3.40)$$

Formula (3.40) shows that the generalized boundary conditions are local in the sense that they do not mix properties of functions in different points.

The explicit expression for the resolvent is

$$(H_{\alpha,Y}^{3d} + \lambda)^{-1} = G^\lambda + \sum_{j,k=1}^n [\Gamma_{\alpha,Y}^{3d}(\lambda)]_{jk}^{-1} G^\lambda(\cdot - y_j) G^\lambda(\cdot - y_k) \quad (3.41)$$

From the analysis of (3.41) one can derive that the continuous spectrum of $H_{\alpha,Y}^{3d}$ is purely absolutely continuous and coincides with the positive real axis. The discrete spectrum consists of (at most) n negative eigenvalues given by the possible solutions $E < 0$ of the equation $\det [\Gamma_{\alpha,Y}^{3d}(-E)] = 0$.

3.2.2 Point interaction in \mathbb{R}^2

With the same approach of the previous section we apply the Krein formula in order to describe point interaction in \mathbb{R}^2 .

For \mathbb{R}^2 the Green function reads:

$$G^z(x) = \frac{i}{4} H_0^{(1)}(k|x-y|) \quad (3.42)$$

here $H_0^{(1)}(\eta)$ is the Bessel function of third kind (also called Hankel function). We recall that $H_0^{(1)}(\eta)$ tends to zero as $|\eta| \rightarrow \infty$ for $\Im\eta > 0$ and that it has a logarithmic singularity in zero

$$H_0^{(1)}(\eta) = \frac{2i}{\pi} \ln \frac{\eta}{2} + 1 + \frac{2i\gamma}{\pi} + \mathcal{O}(\ln(\eta)\eta^2), \quad (3.43)$$

where γ is Euler constant. Following the results contained in [9] (see Theorem 5.2 and 5.3) we can conclude that the family of local point interaction Hamiltonians, with interaction center in $y \in \mathbb{R}^2$, is indexed by a real parameter α and, for each α , has resolvent and domain

$$(H_{\alpha,y}^{2d} - z)^{-1} = (H_0 - z)^{-1} + \frac{2\pi}{2\pi\alpha + \gamma + \ln(k/2i)} \overline{(G^z(\cdot - y), \cdot)} G^z(\cdot - y) \quad (3.44)$$

$$D(H_{\alpha,y}^{2d}) = \left\{ f \in L^2(\mathbb{R}^2) \mid f = \Phi_\lambda + q G_\lambda(\cdot - y), \Phi_\lambda \in H^2(\mathbb{R}^2), q = \frac{2\pi}{2\pi\alpha + \gamma + \ln(k/2i)} \right\} \quad (3.45)$$

where $G_\lambda = G^{z=-\lambda}$.

The action of $H_{\alpha,y}^{2d}$ on $D(H_{\alpha,y}^{2d})$ is easily found to be

$$(H_{\alpha,y}^{2d} - \lambda)f = (-\Delta + \lambda)\Phi_\lambda$$

From the resolvent it is easy to obtain the spectral properties:

$$\sigma(H_{\alpha,y}^{2d}) = [0, \infty) \quad -\infty \leq \alpha \leq \infty$$

$$\sigma(H_{\alpha,y}^{2d}) = \{-4e^{-2[2\pi\alpha+\gamma]}\} \cup [0, \infty) \quad \alpha < 0$$

- for every value of α there is only one simple eigenvalue and the corresponding normalized eigenfunction is

$$\psi_\alpha(x) = -\frac{i}{4} H_0^{(1)} [2ie^{-(2\pi\alpha+\gamma)} |x-y|]$$

- for any $\alpha \in \mathbb{R}$, corresponding to each positive energy E in the continuous spectrum there are infinitely many generalized eigenfunction

$$\Phi_{y,\pm}^{2d}(x, k) = e^{\pm ik \cdot x} + \frac{i\pi/2}{2\pi\alpha + \gamma + \ln(k/2i)} e^{\pm ik \cdot y} H_0^{(1)}(k|x-y|)$$

In [10] an explicit formula for the propagator in this case is given.

Now we give the results for the most general case of n point interactions placed in $Y = \{y_1, \dots, y_n\}$, $y_i \in \mathbb{R}^2$. The family of local point interaction Hamiltonians is indexed by n real constants $\alpha_1, \dots, \alpha_n$ and each Hamiltonian has domain and resolvents given by:

$$D(H_{\alpha,Y}^{2d}) = \left\{ u \in L^2(\mathbb{R}^3) \mid u = \phi^\lambda + \sum_{k=1}^n q_k G_\lambda(\cdot - y_k), \right. \quad (3.46)$$

$$\left. \phi^\lambda \in H^2(\mathbb{R}^2), \phi^\lambda(y_j) = \sum_{k=1}^n [\Gamma_{\alpha,y}^{2d}(\lambda)]_{jk} q_k, j = 1, \dots, n \right\} \quad (3.47)$$

$$(H_{\alpha,Y}^{2d} + \lambda)u = (-\Delta + \lambda)(u - G_Y^\lambda q) \quad (3.48)$$

with

$$G_Y^\lambda q \equiv \sum_{j=1}^n q_j G^\lambda(\cdot - y_j) \quad (3.49)$$

where

$$[\Gamma_{\alpha,Y}^{2d}(\lambda)]_{jk} = \left(2\pi\alpha_j + \gamma + \ln\left(\frac{k}{2i}\right) \right) \delta_{jk} - \tilde{G}^\lambda(y_j - y_k)(1 - \delta_{jk}) \quad (3.50)$$

$$\tilde{G}^\lambda = \begin{cases} G^\lambda(x) & x \neq 0 \\ 0 & x = 0 \end{cases}$$

From the behavior of the function in the point y_j we see that the interaction is local. The explicit expression for the resolvent is

$$(H_{\alpha,Y}^{2d} + \lambda)^{-1} = G^\lambda + \sum_{j,k=1}^n [\Gamma_{\alpha,Y}^{2d}(\lambda)]_{jk}^{-1} G^\lambda(\cdot - y_j) G^\lambda(\cdot - y_k) \quad (3.51)$$

From the analysis of (3.41) one can derive that the continuous spectrum of $H_{\alpha,y}^{2d}$ is purely absolutely continuous and coincides with the positive real axis. The discrete spectrum consists of (at most) n negative eigenvalues given by the possible solutions $E < 0$ of the equation $\det [\Gamma_{\alpha,y}^{2d}(-E)] = 0$.

3.2.3 Point interaction in \mathbb{R}

The Green function in \mathbb{R} reads

$$G^z(x - y) = -\frac{e^{i\sqrt{z}|x-y|}}{2i\sqrt{z}} \quad z \in \mathbb{C} \setminus \mathbb{R}^+, \Im(\sqrt{z}) > 0 \quad (3.52)$$

In $d = 1$ even the derivative of the Green function

$$(G^z)'(x - y) = -\frac{\operatorname{sgn}(x - y)}{2} e^{i\sqrt{z}|x-y|} \quad z \in \mathbb{C} \setminus \mathbb{R}^+, \Im(\sqrt{z}) > 0 \quad (3.53)$$

is in $L^2(\mathbb{R})$. Then $\{G^i, (G^i)'\}$ and $\{G^{-i}, (G^{-i})'\}$ span respectively the deficiency spaces \mathcal{N}^i and \mathcal{N}^{-i} and the deficiency indices of \hat{H} are $(2, 2)$.

Two orthonormal basis of \mathcal{N}^z and $\mathcal{N}^{\bar{z}}$ are $\{g^z, g_1^z\}$ and $\{g^{\bar{z}}, g_1^{\bar{z}}\}$ respectively where

$$g^z(x - y) = \frac{G^z(x - y)}{\|G^z\|} = i \frac{\sqrt{|z|} \Im(\sqrt{z})}{\sqrt{z}} e^{i\sqrt{z}|x-y|} \quad (3.54)$$

$$g_1^z(x - y) = \frac{(G^z)'(x - y)}{\|(G^z)'\|} = -\sqrt{\Im(\sqrt{z})} \operatorname{sgn}(x - y) e^{i\sqrt{z}|x-y|} \quad (3.55)$$

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

Following the von Neumann construction we have that if U is a unitary application from \mathcal{N}^i to \mathcal{N}^{-i} , operator H^U defined by

$$D(H^U) = \left\{ \psi : \psi = \psi_0 + c_1 g^i + c_2 g_1^i + c'_1 g^{-i} + c'_2 g_1^{-i}; \psi_0 \in D(\hat{H}), \right. \\ \left. c_1, c_2 \in \mathbb{C}, c'_m = \sum_{n=1,2} U_{mn} c_n, m = 1, 2 \right\} \quad (3.56)$$

$$H^U \psi = \hat{H} \psi_0 + i(c_1 g^i + c_2 g_1^i - c'_1 g^{-i} - c'_2 g_1^{-i}) \quad (3.57)$$

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 .

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

$$U = \begin{pmatrix} -e^{i\theta} \cos \omega & e^{i(\theta+\rho)} \sin \omega \\ -e^{i(\varphi-\rho)} \sin \omega & -e^{i\varphi} \cos \omega \end{pmatrix} \quad (3.58)$$

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

Following the results of [26] we have a classification of the selfadjoint extensions depending on the value of the parameters in the matrix U .

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

$$D(H_0) = \left\{ \psi : \psi = \psi_0 + c_1(g^i - g^{-i}) + c_2(g_1^i - g_1^{-i}); \right. \\ \left. \psi_0 \in D(\hat{H}), c_1, c_2 \in \mathbb{C} \right\} \quad (3.59)$$

$$H_0 \psi = \hat{H} \psi_0 + i(c_1(g^i + g^{-i}) + c_2(g_1^i + g_1^{-i})). \quad (3.60)$$

Functions in the domain of H_0 are continuous and have continuous derivative in y , from its definition the operator H_0 coincides with the “free” Hamiltonian i.e.

$$D(H_0) = H^2(\mathbb{R}) \quad H_0\psi = -\frac{d^2}{dx^2}\psi \quad \psi \in D(H_0). \quad (3.61)$$

Operator $H_{\alpha,y}^{1d} = -\Delta + \alpha\delta_y$ is given by $\omega = \varphi = 0$, and the domain is written as

$$D(H_{\alpha,y}^{1d}) = \left\{ \psi \in H^1(\mathbb{R}) \cap H^2(\mathbb{R} \setminus \{y\}) : \right. \\ \left. \psi'(y^+) - \psi'(y^-) = \alpha\psi(y), \quad -\infty < \alpha \leq \infty \right\} \quad (3.62)$$

$$H_{\alpha,y}^{1d} = -\frac{d^2}{dx^2}. \quad (3.63)$$

with α is related to θ by formula

$$\alpha = \frac{\sqrt{2}(\cos \theta + \sin \theta - 1)}{1 - \sin \theta} \quad (3.64)$$

Interaction given by Hamiltonian $H_{\alpha,y}^{1d}$ is often referred to as δ -interaction. We indicate with $H_{\beta,y}^{1d}$ the other extension of H_0 given by $\omega = \theta = 0$, and the domain is

$$D(H_{\beta,y}^{1d}) = \left\{ \psi \in H^2(\mathbb{R} \setminus \{y\}) : \psi'(y^+) = \psi'(y^-), \right. \\ \left. \psi(y^+) - \psi(y^-) = \beta\psi'(y), \quad -\infty < \beta \leq \infty \right\} \quad (3.65)$$

$$H_{\beta,y}^{1d} = -\frac{d^2}{dx^2}. \quad (3.66)$$

Constant β is related to φ by formula

$$\beta = \frac{\sqrt{2}(\cos \varphi - \sin \varphi - 1)}{1 + \sin \varphi} \quad (3.67)$$

Interaction given by Hamiltonian $H_{\beta,y}^{1d}$ is often referred to as δ' -interaction. In order to obtain the spectrum is preferable to describe the point interaction with the Krein formula for the resolvent (3.14).

We indicate with H^Θ the generic self-adjoint extension of H , usually it is useful to express the resolvent of H^Θ with respect to the “free” resolvent $(H_0 - z)^{-1}$:

$$(H^\Theta - z)^{-1} = (H_0 - z)^{-1} + \sum_{m,n=1,2} (\Gamma(z))_{mn}^{-1} (\phi_n^{\bar{z}}, \cdot) \phi_m^z \quad z \in \rho(H^\Theta) \quad (3.68)$$

where functions ϕ_m^z are defined by

$$\phi_1^z(x) = G^z(x - y); \quad \phi_2^z(x) = (G^z)'(x - y) \quad z \in \mathbb{C} \setminus \mathbb{R}^+ \quad (3.69)$$

By direct calculation one can check that ϕ_m^z satisfy relation

$$\phi_m^z = \phi_m^{z_0} + (z - z_0)(H_0 - z)^{-1}\phi_m^{z_0} \quad m = 1, 2; \quad z, z_0 \in \rho(H_0) \quad (3.70)$$

Matrix $\Gamma(z)$ is defined by

$$\Gamma(z)_{mn} - \Gamma(z')_{mn} = (z' - z)(\phi_n^{\bar{z}}, \phi_m^{z'}) \quad m, n = 1, 2; \quad z, z' \in \rho(H^\Theta) \quad (3.71)$$

and

$$\Gamma(z)^* = \Gamma(\bar{z}) \quad z \in \rho(H^\Theta) \quad (3.72)$$

Functions $\Gamma(z)_{mn}$ and ϕ_m^z , are analytic in $z \in \rho(H^\Theta)$, notice that $\rho(H^\Theta) \subseteq \rho(\hat{H})$. Relation (3.71) does not define univocally the matrix $\Gamma(z)$, by direct calculation one can verify that

$$\Gamma(z) = \begin{pmatrix} \frac{1}{2i\sqrt{z}} & 0 \\ 0 & \frac{\sqrt{z}}{2i} \end{pmatrix} + \Theta, \quad (3.73)$$

where Θ is a 2×2 arbitrary, constant, Hermitian matrix, satisfies conditions (3.71) and (3.72). Then the resolvent is found by inverting the matrix $\Gamma(z)$ and by formula (3.68). 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 $H_{\alpha,y}^{1d}$.

The maximal common part is

$$\ddot{H} = -\frac{d^2}{dx^2}, \quad D(\ddot{H}) = \{\psi \in H^2(\mathbb{R}) : \psi(y) = 0\}, \quad (3.74)$$

its adjoint is

$$\ddot{H}^* = -\frac{d^2}{dx^2}, \quad D(\ddot{H}^*) = H^2(\mathbb{R} \setminus \{y\}) \cap H^1(\mathbb{R}). \quad (3.75)$$

Then the only independent solution of equation

$$(\hat{H}^* - z)\phi^z = 0 \quad \phi^z \in L^2(\mathbb{R}), \quad z \in \mathbb{C} \setminus \mathbb{R} \quad (3.76)$$

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

$$\Gamma(z) = \frac{1}{2i\sqrt{z}} - \frac{1}{\alpha} \quad (3.77)$$

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

$$\Gamma(z) - \Gamma(z') = (z' - z)(G^{\bar{z}}, G^{z'}) \quad z, z' \in \rho(H_\alpha^{1d}) \quad (3.78)$$

and

$$\overline{\Gamma(z)} = \Gamma(\bar{z}) \quad z \in \rho(H_\alpha^{1d}) \quad (3.79)$$

Then resolvent of $H_{\alpha,y}^{1d}$ can be written as

$$(H_{\alpha,y}^{1d} - z)^{-1} = (H_0 - z)^{-1} - \frac{2\alpha\sqrt{z}}{i\alpha + 2\sqrt{z}} (G^{\bar{z}}(\cdot - y), \cdot) G^z(\cdot - y) \quad (3.80)$$

$$z \in \rho(H_{\alpha}^{1d})$$

and operator $H_{\alpha,y}^{1d}$ can be defined as

$$D(H_{\alpha,y}^{1d}) = \left\{ \psi \in L^2(\mathbb{R}) : \psi = \psi^z - \frac{2\alpha\sqrt{z}}{i\alpha + 2\sqrt{z}} \psi^z(y) G^z(\cdot - y); \right. \quad (3.81)$$

$$\left. \psi^z \in D(H), z \in \rho(H_{\alpha,y}^{1d}), \Im\sqrt{z} > 0 \right\}$$

$$(H_{\alpha,y}^{1d} - z)\psi = (H - z)\psi^z \quad (3.82)$$

Function ψ^z is called regular part of ψ , if $\psi^z(y) = 0$ then $\psi = \psi^z$ and $H_{\alpha,y}^{1d}\psi = H\psi$. Starting from formula (3.81) it is easy to verify that functions in $D(H_{\alpha,y}^{1d})$ satisfy boundary condition

$$\psi'(y^+) - \psi'(y^-) = \alpha\psi(y) \quad (3.83)$$

An exhaustive analysis of all the singular perturbations of $-\Delta$ in one dimension is in [10].

From the resolvent it is easy to obtain the spectral properties for a δ interaction in \mathbb{R} .

$$\sigma(H_{\alpha,y}^{1d}) = [0, \infty) \quad \alpha \geq 0$$

$$\sigma(H_{\alpha,y}^{1d}) = \left\{ -\frac{\alpha^2}{4} \right\} \cup [0, \infty) \quad \alpha < 0$$

- for $\alpha < 0$ the only eigenvalue is simple and the corresponding normalized eigenfunction is

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

- for any $\alpha \in \mathbb{R}$, corresponding to each positive energy E in the continuous spectrum there are infinitely many generalized eigenfunction

$$\Phi_{y,\pm}^{1d}(x, k) = e^{\pm ik \cdot x} - \frac{\alpha}{\alpha - 2i|k|} e^{\pm ik \cdot y} e^{i|k||x-y|}$$

In the article [10] is contained an explicit formula for the propagator in the one dimensional case for a δ like interaction.

The generalization to a finite or infinite number of points is contained in [9].

Now we give only the results for point interactions placed at $Y = \{y_1, \dots, y_n\}$ $y_i \in \mathbb{R}$ with parameters of interaction $\alpha = \{\alpha_1, \dots, \alpha_n\}$, $\alpha_i \in \mathbb{R}$. The domain and the action of $H_{\alpha, Y}^{1d}$, the selfadjoint operator expressing point interaction in Y , are

$$D(H_{\alpha, Y}^{1d}) = \{u \in H^1(\mathbb{R}) \cap H^2(\mathbb{R} \setminus \{y_1, \dots, y_n\}) \mid u'(y_j^+) - u'(y_j^-) = \alpha_j u(y_j), j = 1, \dots, n\} \quad (3.84)$$

$$(H_{\alpha, Y}^{1d} + \lambda)u = (-\Delta + \lambda) \left(u - \sum_{j=1}^n q_j^{1d} G^\lambda(\cdot - y_j) \right) \quad (3.85)$$

where $\lambda > 0$, $q_j^{1d} = -\alpha_j u(y_j)$ and $G^\lambda(x - x')$ is the Green's function of the free laplacian

The domain (3.84) consists of functions belonging to the domain of the free laplacian except at the position of the interactions, where the derivative has a jump and a boundary condition is satisfied. In fact it is easy to see that each element of the domain can be represented as $u = \phi^\lambda + \sum_{j=1}^n q_j^{1d} G^\lambda(\cdot - y_j)$, where $\phi^\lambda \equiv u - \sum_{j=1}^n q_j^{1d} G^\lambda(\cdot - y_j) \in H^2(\mathbb{R})$.

If the operator (3.85) is applied to a smooth function u vanishing at y_1, \dots, y_n then it reduces to the free laplacian.

The solution of a standard boundary value problem for the laplacian on the real line yields to the explicit expression for the resolvent

$$(H_{\alpha, y}^{1d} + \lambda)^{-1} = G^\lambda + \sum_{j, k=1}^n [\Gamma_{\alpha, y}^{1d}(\lambda)]_{jk}^{-1} G^\lambda(\cdot - y_j) G^\lambda(\cdot - y_k) \quad (3.86)$$

where

$$[\Gamma_{\alpha, y}^{1d}(\lambda)]_{jk} = \alpha_j^{-1} \delta_{jk} + G^\lambda(y_j - y_k)(1 - \delta_{jk}) \quad (3.87)$$

All the spectral properties of (3.85) can be easily derived from the resolvent (3.86). We simply list them.

The continuous spectrum is purely absolutely continuous and coincides with the positive real axis. Moreover there are at most n negative eigenvalues given by the possible solutions $E < 0$ of the equation $\det [\Gamma_{\alpha, y}^{1d}(-E)] = 0$.

The proper and the generalized eigenfunctions can also be explicitly computed.

Chapter 4

A model of scattering based on point interaction

In this section we give a rigorous treatment of the asymptotic dynamics of a quantum particle undergoing a single scattering event with a much lighter particle. As seen in the previous chapter the knowledge of such a process is the necessary preliminary step for the formulation of a realistic model for the dynamics of a quantum particle evolving in an environment made up of many light particles.

The Joos and Zeh formula, discussed in detail in chapter 2, states that, in the roughest approximation, the scattering process is described by the instantaneous transition

$$\varphi(R)\chi(r) \rightarrow \varphi(R) (S^R\chi) (r) \quad (4.1)$$

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 was analyzed in a series of papers ([39], [38] and [5]) for different models of two body interaction. In [38] and [5] 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 potential in three dimensions. Their results can be considered as a rigorous formulation of the Joos and Zeh formula (4.1).

In this section we will 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. The “free” Hamiltonian describing two non interacting

particles of mass M and m is the operator

$$D(H_0) = H^2(\mathbb{R}^3, dR) \otimes H^2(\mathbb{R}^3, dr) \quad H_0 = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2m}\Delta_r. \quad (4.2)$$

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 $\hbar = 1$ and we define $\varepsilon \equiv \frac{m}{M}$. At formal level the operator (4.2) can be written as

$$H_0^\varepsilon = H_0 \otimes \frac{1}{\varepsilon}H_0 \quad (4.3)$$

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 for a three dimensional system of two particles interacting via point interaction in $L^2(\mathbb{R}^3, dx) \otimes L^2(\mathbb{R}^3, dy)$ reads

$$H^\varepsilon = H_0^\nu \otimes H_\alpha^\mu \quad (4.4)$$

where $\nu = (1 + \varepsilon)$ is the total mass of the system, $\mu = \frac{\varepsilon}{1+\varepsilon}$ is the reduced mass and H_0^ν indicates the free Hamiltonian relative to a particle of mass ν and coordinate x and H_α^μ is a point interaction Hamiltonian for a particle of mass μ . Notice that in (4.4) with H_α^μ we mean $\frac{1}{\mu}H_\alpha$ suggesting that a rescaling of the coupling constant α has been made (compare with the cases of two body potentials [38] and [5]).

We consider the problem

$$i\frac{\partial\Psi^\varepsilon(t)}{\partial t} = H^\varepsilon\Psi^\varepsilon(t) \quad (4.5)$$

$$\Psi^\varepsilon(0; R, r) = \varphi(R)\chi(r) \quad (4.6)$$

in the limit of small ε .

The initial conditions (4.6) states that 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.

Our main result is expressed in the following theorem where we indicate with $\|\cdot\|$ the $L^2(\mathbb{R}^6)$ -norm.

Theorem 4.0.1. *There exist two constants $A > 0$ and $B > 0$ such that for any initial state (4.6) and any fixed $\alpha > 0$ and $t > 0$, one has*

$$\|\Psi^\varepsilon(t) - \Psi^a(t)\| \leq A\left(\frac{\varepsilon}{t}\right)^{\frac{3}{4}} + B\varepsilon \quad (4.7)$$

where

$$\Psi^a(t) = e^{-itH_0^\varepsilon} \Psi_0^a \quad (4.8)$$

$$H_0^\varepsilon = H_0 \otimes \frac{1}{\varepsilon} H_0 \quad (4.9)$$

$$\Psi_0^a(R, r) = \varphi(R) \left[(\Omega_+^R)^{-1} \chi \right] (r) \quad (4.10)$$

and the constants A and B depend only on the initial state (see below for details) and on the constant α .

The result of theorem 4.0.1 expressed by (4.8), (4.9), (4.10) can be thought as an exact formulation of the Joos and Zeh conjecture (4.1) for the special case of point interactions in three dimensions. As stressed by many authors (see e.g. [85], [52], [38], [5],) formula (4.1) 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 (4.10) shows that the approximation formula holds true if in (4.1) the scattering matrix S^R is replaced with the wave operator $(\Omega_+^R)^{-1}$

The proof of the theorem is contained in the Appendix A

4.1 Decoherence induced by scattering

We want to apply the results contained in theorem 4.0.1 to the analysis of the decoherence effects induced by a single scattering event.

The often called “naive” interpretation of decoherence in quantum systems that we introduced in the last chapter will be the main idea behind the considerations which follow. Roughly speaking that interpretation insists on the almost obvious statement that entanglement causes a diffusion of quantum correlations out of every subsystem in interaction with a large environment.

We recall that the mechanism is essentially described as follows: suppose to have a subsystem of a large system which is initially in a pure state. Entanglement induced by the interaction of the subsystem with its environment forces the quantum correlations between local observables to migrate into the whole system. Trace over the exterior degrees of freedom partially cancels correlations making the reduced density matrix, describing the evolution of the subsystem, a statistical mixture.

In the following we will find an estimate for the effect of decoherence resulting from 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 [38], 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 $\rho^\varepsilon(t)$ in $L^2(\mathbb{R}^3)$ with $\text{Tr} \rho^\varepsilon(t) = 1$ with integral kernel

$$\rho^\varepsilon(t; R, R') = \int_{\mathbb{R}^3} dr \Psi^\varepsilon(t; R, r) \overline{\Psi^\varepsilon(t; R', r)} \quad (4.11)$$

where $\Psi^\varepsilon(t; R, r)$ is the solution of problem (4.5), (4.6).

In the small mass ratio limit, using the results contained in theorem 4.0.1, one easily obtains the following approximation for the density matrix (4.11)

$$\rho^a(t) = e^{-itH_0} \rho_0^a e^{itH_0} \quad (4.12)$$

where

$$\rho_0^a(R, R') = \varphi(R) \overline{\varphi(R')} \mathcal{I}(R, R') \quad (4.13)$$

$$\mathcal{I}(R, R') = ((\Omega_+^R)^{-1} \chi, (\Omega_+^{R'})^{-1} \chi) \quad (4.14)$$

It is easily seen that the following proposition holds

Proposition 1. *Under the same assumptions of the theorem 4.0.1 one has*

$$\text{Tr} |\rho^\varepsilon(t) - \rho^a(t)|^{\frac{1}{2}} \leq A \left(\frac{\varepsilon}{t}\right)^{\frac{3}{4}} + B\varepsilon \quad (4.15)$$

Without interaction the dynamics of the heavy particle is described by 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

$$\text{Tr}(\rho(t))^2 = \text{Tr}(\rho_0)^2 = 1 \quad (4.16)$$

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

$$\text{Tr}(\rho^a(t))^2 = \text{Tr}(\rho_0^a)^2 < 1 \quad (4.17)$$

which in turns means that the reduced density matrix (4.12) 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

$$\mathcal{I}(R, R') = (\mathcal{F}_+^R \chi, \mathcal{F}_+^{R'} \chi) \quad (4.18)$$

We introduce the notation

$$\mathcal{F}_+^R = \mathcal{F} + K_R \quad (4.19)$$

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

$$[K_R \chi](|k|) = \int_{\mathbb{R}^3} \frac{dr}{(2\pi)^{\frac{3}{2}}} \frac{e^{-ikR}}{4\pi\alpha - i|k|} \frac{e^{i|k||r-R|}}{|r-R|} \chi(r) \quad (4.20)$$

with this notation

$$\mathcal{I}(R, R') = (\chi, \chi) + (K_R \chi, \mathcal{F} \chi) + (\mathcal{F} \chi, K_{R'} \chi) + (K_R \chi, K_{R'} \chi) \quad (4.21)$$

Notice that because the unitarity of $(\Omega_+^R)^{-1}$, $\mathcal{I}(R, R) = (\chi, \chi)$ and (4.21) implies

$$(K_R \chi, \mathcal{F} \chi) = -(\mathcal{F} \chi, K_R \chi) - (K_R \chi, K_R \chi) \quad (4.22)$$

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 (4.21) and (4.22) we obtain

$$1 - \mathcal{I}(R, R') = (\mathcal{F} \chi, (K_R - K_{R'}) \chi) + (K_R \chi, (K_R - K_{R'}) \chi) \quad (4.23)$$

We will analyze (4.23) 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

$$\chi(r) = \frac{e^{-\frac{|r|^2}{2\sigma^2}}}{(\pi\sigma^2)^{\frac{3}{4}}} \quad (4.24)$$

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 $\chi(r) = \chi(-r)$

$$(\mathcal{F} \chi, (K_R - K_{-R}) \chi) = 0 \quad (4.25)$$

Under the same assumption on $\chi(r)$ the second term in the r.h.s. of (4.23) can be written as

$$\begin{aligned}
& (K_R \chi, (K_R - K_{-R}) \chi) = \\
& = \int_{\mathbb{R}^3} \frac{dk}{(2\pi)^3} \frac{1 - e^{2ikR}}{(4\pi\alpha)^2 + |k|^2} \int_{\mathbb{R}^3} dr \frac{e^{-i|k||r|}}{|r|} \bar{\chi}(r+R) \int_{\mathbb{R}^3} dr' \frac{e^{i|k||r'|}}{|r'|} \chi(r'+R) \quad (4.26)
\end{aligned}$$

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 (4.24) of $\chi(r)$ we obtain

$$\begin{aligned}
& \left| \int dr \frac{e^{-i|k||r|}}{|r|} \bar{\chi}(r+R) \right|^2 = \\
& = 2\pi^{\frac{3}{2}} \frac{\sigma^3}{|R|^2} e^{-|k|^2\sigma^2} \left| e^{i|k||R|} \operatorname{erf}(z) + e^{-i|k||R|} \overline{\operatorname{erf}(z)} - 2i \sin |k||R| \right|^2 \quad (4.27)
\end{aligned}$$

where $z = \frac{|R|+i|k|\sigma^2}{\sqrt{2}\sigma}$. Inserting this in (4.26) and integrating on the angular part of k we have

$$\begin{aligned}
1 - \mathcal{I}(R, -R) &= \frac{\sigma^3}{|R|^2 \sqrt{\pi}} \int_0^\infty dk \frac{|k|^2}{(4\pi\alpha)^2 + |k|^2} \left(1 - \frac{\sin(2|k||R|)}{2|k||R|} \right) e^{-|k|^2\sigma^2} \times \\
& \times \left| e^{i|k||R|} \operatorname{erf}(z) + e^{-i|k||R|} \overline{\operatorname{erf}(z)} - 2i \sin |k||R| \right|^2 \quad (4.28)
\end{aligned}$$

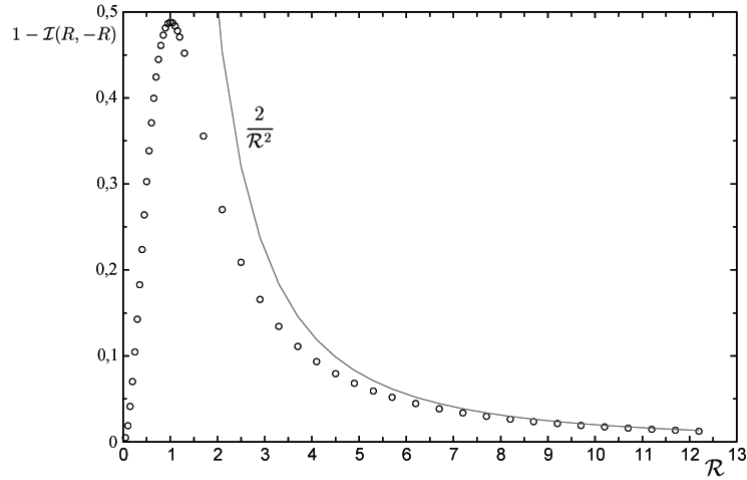
Expression (4.28) clearly shows that for every R one has $1 - \mathcal{I}(R, -R) \geq 0$, moreover it is easy to see that, for fixed R , $1 - \mathcal{I}(R, -R)$ is a decreasing function of α . For this reason we focus our attention on the evaluation of (4.28) when $\alpha = 0$.

We define the dimensionless variables $\xi \equiv |k||R|$ and $\mathcal{R} \equiv \frac{|R|}{\sigma}$. With this notation one has

$$\begin{aligned}
1 - \mathcal{I}(R, -R) &= \frac{1}{|\mathcal{R}|^3 \sqrt{\pi}} \int_0^\infty d\xi \left(1 - \frac{\sin(2\xi)}{2\xi} \right) e^{-\frac{\xi^2}{\mathcal{R}^2}} \times \\
& \times \left| e^{i\xi} \operatorname{erf} \left(\frac{\mathcal{R}}{\sqrt{2}} + \frac{i}{\sqrt{2}} \frac{\xi}{\mathcal{R}} \right) + e^{-i\xi} \operatorname{erf} \left(\frac{\mathcal{R}}{\sqrt{2}} - \frac{i}{\sqrt{2}} \frac{\xi}{\mathcal{R}} \right) - 2i \sin \xi \right|^2 \quad (4.29)
\end{aligned}$$

Analyzing the asymptotics of the positive integral in (4.29) it is easy to check that $1 - \mathcal{I}(R, -R)$ 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 (4.29) 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 (4.24) 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 approximatively given by the classical flight time $\frac{|R|}{|p_0|}$ one expects quantum interference to take place for distances of the order of the dispersion of the two wave packets.

Formula (4.13) 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.

As it was discussed in the last chapter many authors 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 (4.0.1) in the direction suggested by the Joos and Zeh formula. 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.

Part II

Particle-Spin interaction

Chapter 5

Interaction

5.1 Introduction

At the end of the last chapter we stressed the difficulties one encounters in investigating the Schrödinger dynamics of a set of particles when their number exceeds two. In order to have models of a multipartite environment we should consider an array of simple quantum systems interacting with the test particle. In this chapter we construct models for the dynamics of one quantum particle in interaction with any number of localized spins. In this way we are able to define simple, but genuinely multi-component, quantum systems where conjectures and qualitative results in the theory of quantum open systems can, in principle, be rigorously approached.

For the sake of simplicity we examine systems consisting of one spinless particle in interaction with localized $1/2$ spins (in units where $\hbar = 1$).

Physical phenomenology would suggest considering the particle with spin and a spin-spin interaction conserving the total spin. It is easy to convince oneself that, in the latter case, inside each channel characterized by a fixed value of the total spin, the dynamics would be described by some Hamiltonian of the type we consider here, possibly relative to a value of the spin larger than $1/2$. Few examples of such Hamiltonians were already heuristically found and used to study different problems, e.g., the spin dependent scattering [65] or the interaction of one quantum particle with one or (several) quantum dots [14]. The straightforward generalization to higher values of the spin will not be given here.

In Section 5.2.1 we introduce some notation and define the free quantum dynamics for the particle and the spins. In Section 5.2.2 we state and prove our main results: we give a complete characterization of all zero-range perturbations of the free dynamics in any dimension. At the end of Section 5.2.2 we discuss with more detail two examples of spin-dependent point interactions that, in our opinion, are of interest as non trivial solvable models. In order to

make clearer our formulas, the resolvent in the simple case of $N = 1$ and $d = 3$ is written in an extended form.

5.2 Particle-Spin interaction

5.2.1 Some notation and the free dynamics

In this section we define the state space for a quantum system consisting of one particle and an array of N spins. Moreover we introduce some notation and define the non-interacting Hamiltonian H_0 .

We will consider here the case of spin 1/2. The state of each spin placed in a fixed position of space is represented by a unitary vector in \mathbb{C}^2 .

Consider the first Pauli matrix, $\hat{\sigma}_j^{(1)}$, where the index $j = 1, \dots, N$ indicates that such operator refers to the j -th spin. We indicate with χ_{σ_j} the normalized eigenvector of the operator $\hat{\sigma}_j^{(1)}$ with eigenvalue $\sigma_j = \pm 1$

$$\hat{\sigma}_j^{(1)} \chi_{\sigma_j} = \sigma_j \chi_{\sigma_j} \quad \sigma_j = \pm 1; \quad \|\chi_{\sigma_j}\|_{\mathbb{C}^2} = 1; \quad j = 1, \dots, N. \quad (5.1)$$

With this notation the state of the j -th spin can be written as the linear superposition $a_j \chi_+ + b_j \chi_-$, with $a_j, b_j \in \mathbb{C}$ and $|a_j|^2 + |b_j|^2 = 1$.

The natural Hilbert space for the description of a system of one particle in dimension d and N spins 1/2 is then

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathbb{S}_N, \quad (5.2)$$

where

$$\mathbb{S}_N = \overbrace{\mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2}^N \quad (5.3)$$

We consider the cases $d = 1, 2, 3$. We indicate with a capital Greek letter a generic vector in \mathcal{H} .

Let us define $\mathcal{X}_{\underline{\sigma}} = \chi_{\sigma_1} \otimes \dots \otimes \chi_{\sigma_N}$, where $\underline{\sigma}$ is the N -dimensional vector $\underline{\sigma} = (\sigma_1, \dots, \sigma_N)$. Trivially $\mathcal{X}_{\underline{\sigma}} \in \mathbb{S}_N$, $\|\mathcal{X}_{\underline{\sigma}}\|_{\mathbb{S}_N} = 1$ and the following decomposition formula holds

$$\Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \quad \Psi \in \mathcal{H}, \quad (5.4)$$

where the sum runs over all the possible configurations of the vector $\underline{\sigma}$ while $\psi_{\underline{\sigma}} \in L^2(\mathbb{R}^d) \forall \underline{\sigma}$ is referred to as the wave function component of the state Ψ . The choice of the $\mathcal{X}_{\underline{\sigma}}$ as basis of \mathbb{S}_N is arbitrary, we consider the basis of eigenvectors of $\hat{\sigma}_j^{(1)}$ according to what will be our choice for the free Hamiltonian.

The scalar product in \mathcal{H} is defined in a natural way by

$$\langle \Psi, \Phi \rangle = \sum_{\underline{\sigma}} (\psi_{\underline{\sigma}}, \phi_{\underline{\sigma}})_{L^2} \quad \Psi, \Phi \in \mathcal{H}. \quad (5.5)$$

Consider the operator in \mathbb{S}_N

$$\mathbf{S}_j = \overbrace{\mathbb{I}_{\mathbb{C}^2} \otimes \dots \otimes \hat{\sigma}_j^{(1)} \otimes \dots \otimes \mathbb{I}_{\mathbb{C}^2}}^N \quad j = 1, \dots, N. \quad (5.6)$$

Vectors $\mathcal{X}_{\underline{\sigma}}$ are eigenvectors of \mathbf{S}_j ,

$$\mathbf{S}_j \mathcal{X}_{\underline{\sigma}} = \sigma_j \mathcal{X}_{\underline{\sigma}} \quad j = 1, \dots, N. \quad (5.7)$$

The following operator is self-adjoint in \mathcal{H}

$$D(H_0) = H^2(\mathbb{R}^d) \otimes \mathbb{S}_N \quad (5.8)$$

$$H_0 = -\frac{\hbar^2}{2m} \Delta \otimes \mathbb{I}_{\mathbb{S}_N} + \sum_{j=1}^N \mathbb{I}_{L^2} \otimes \beta_j \mathbf{S}_j \quad \beta_j \in \mathbb{R}, \quad (5.9)$$

here $H^2(\mathbb{R}^d)$ indicates the standard Sobolev space of functions in $L^2(\mathbb{R}^d)$, m indicates the mass of the particle and β_j are real constants with the dimension of an energy. The operator H_0 defines the free Hamiltonian. In the following we will fix $\hbar = 1$ and $2m = 1$.

By using the decomposition formula (5.4) it is easily seen that the action of H_0 on vectors in its domain is given by

$$H_0 \Psi = \sum_{\underline{\sigma}} (-\Delta + \underline{\beta} \underline{\sigma}) \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \quad \Psi \in \mathcal{H}, \quad (5.10)$$

where $\underline{\sigma}$ is the N -dimensional real vector $(\beta_1, \dots, \beta_N)$ and $\underline{\beta} \underline{\sigma} = \sum_{j=1}^N \beta_j \sigma_j$. The resolvent of H_0 , $R(z) = (H_0 - z)^{-1}$, is

$$R(z) \Psi = \sum_{\underline{\sigma}} (-\Delta - z + \underline{\beta} \underline{\sigma})^{-1} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \quad \Psi \in \mathcal{H}; \quad z \in \rho(H), \quad (5.11)$$

where $\rho(H_0)$ indicates the resolvent set of H_0 . We indicate with $G^w(x - x')$ the integral kernel of the operator $(-\Delta - w)^{-1}$. Its explicit expression is well known and reads

$$G^w(x) := \begin{cases} i \frac{e^{i\sqrt{w}|x|}}{2\sqrt{w}} & d = 1 \\ \frac{i}{4} H_0^{(1)}(\sqrt{w}|x|) & d = 2 \\ \frac{e^{i\sqrt{w}|x|}}{4\pi|x|} & d = 3 \end{cases} \quad \text{with } w \in \mathbb{C} \setminus \mathbb{R}^+; \quad \Im(\sqrt{w}) > 0 \quad (5.12)$$

From the spectral properties of the operator $-\Delta$, with domain $D(-\Delta) = H^2(\mathbb{R}^d)$, it is easily seen that the spectrum of H_0 is only absolutely continuous, in particular

$$\sigma_{pp}(H) = \emptyset; \quad \sigma_{ess}(H) = \sigma_{ac}(H) = [\mu, \infty), \quad \mu = \min_{\underline{\sigma}}(\underline{\beta} \underline{\sigma}). \quad (5.13)$$

The solution of the Schrödinger equation

$$i\frac{d}{dt}\Psi^t = H_0\Psi^t, \quad (5.14)$$

with initial datum

$$\Psi^{t=0} = \Psi^0 = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}}^0 \otimes \mathcal{X}_{\underline{\sigma}} \quad \Psi^0 \in \mathcal{H}, \quad (5.15)$$

is formally written as $e^{-itH_0}\Psi_0$. By using the property of the Laplace transform $\mathcal{L}^{-1}\left(\mathcal{L}(f)(\cdot+s)\right)(\tau) = e^{s\tau}f(\tau)$ we obtain the strongly continuous unitary group e^{-itH_0} (see, e.g., Th. VIII.7 [75])

$$\Psi^t = e^{-iH_0t}\Psi^0 = \sum_{\underline{\sigma}} U^t \psi_{\underline{\sigma}}^0 \otimes e^{-i\beta_{\underline{\sigma}}t} \mathcal{X}_{\underline{\sigma}}, \quad (5.16)$$

where $U^t : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ is the generator of the free dynamics for one particle in d dimensions

$$(U^t f)(x) = \frac{1}{(4\pi it)^{d/2}} \int_{\mathbb{R}^d} e^{i\frac{|x-x'|^2}{4t}} f(x') dx'. \quad (5.17)$$

The Hamiltonian H_0 does not give rise to any interaction among the particle and the spins and of the spins among themselves.

5.2.2 Point perturbations of H

In this section we use the theory of self-adjoint extensions of symmetric operators to derive the whole family of Hamiltonians that coincide with H on functions whose support does not contain the set of points where the spins are placed with the same approach followed in section 3.2 (see also [6] and [76]). Let us indicate with Y the set $\{y_1, \dots, y_N\}$, where $y_j \in \mathbb{R}^d$ indicates the position of the j -th spin $1/2$. Consider the symmetric operator on \mathcal{H}

$$D(\hat{H}) = C_0^\infty(\mathbb{R}^d \setminus Y) \otimes \mathbb{S}_N \quad (5.18)$$

$$\hat{H} = -\Delta \otimes \mathbb{I}_{\mathbb{S}_N} + \sum_{j=1}^N \mathbb{I}_{L^2} \otimes \alpha_j \mathbf{S}_j \quad \alpha_j \in \mathbb{R} \quad (5.19)$$

Let $\mathcal{N}_z(\hat{H}) = \text{Ker}[\hat{H}^* - z]$ with $\Im(z) \neq 0$, where $*$ indicates the adjoint. To evaluate the deficiency indices of \hat{H} , $n_+(\hat{H}) = \dim[\mathcal{N}_i]$ and $n_-(\hat{H}) = \dim[\mathcal{N}_{-i}]$, we have to find all the independent solutions of the equation

$$(\hat{H}^* - z)\Phi^z = 0 \quad z \in \mathbb{C} \setminus \mathbb{R}; \quad \Phi^z \in D(\hat{H}^*). \quad (5.20)$$

Define $\Phi^z = \sum_{\underline{\sigma}} \phi_{\underline{\sigma}}^z \otimes \mathcal{X}_{\underline{\sigma}}$, then equation (5.20) is equivalent to

$$\left(\phi_{\underline{\sigma}}^z, (-\Delta - \bar{z} + \underline{\beta}_{\underline{\sigma}}) \psi \right)_{L^2} = 0 \quad \phi_{\underline{\sigma}}^z \in L^2(\mathbb{R}^d); \forall \psi \in C_0^\infty(\mathbb{R}^d \setminus Y); z \in \mathbb{C} \setminus \mathbb{R}. \quad (5.21)$$

The independent solutions of (5.20) in \mathcal{H} are

$$\begin{cases} \Phi_{0j\underline{\sigma}}^z = G^{z-\underline{\beta}_{\underline{\sigma}}}(\cdot - y_j) \otimes \mathcal{X}_{\underline{\sigma}} \\ \Phi_{1j\underline{\sigma}}^z = (G^{z-\underline{\beta}_{\underline{\sigma}}})'(\cdot - y_j) \otimes \mathcal{X}_{\underline{\sigma}} \end{cases} \quad z \in \mathbb{C} \setminus \mathbb{R} \quad d = 1 \quad (5.22)$$

$$\Phi_{j\underline{\sigma}}^z = G^{z-\underline{\beta}_{\underline{\sigma}}}(\cdot - y_j) \otimes \mathcal{X}_{\underline{\sigma}} \quad z \in \mathbb{C} \setminus \mathbb{R} \quad d = 2, 3 \quad (5.23)$$

where $G^w(x)$, $w \in \mathbb{C} \setminus \mathbb{R}^+$, is defined in (5.12).

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

$$(G^w)'(x) = -\text{sgn}(x) \frac{e^{i\sqrt{w}|x|}}{2} \quad w \in \mathbb{C} \setminus \mathbb{R}^+; \Im(\sqrt{w}) > 0 \quad d = 1 \quad (5.24)$$

Since the index $\underline{\sigma}$ runs over 2^N distinct configurations and $j = 1, \dots, N$, for $d = 1$ the deficiency indices are $n_+ = n_- = N2^{N+1}$ while for $d = 2, 3$ one has $n_+ = n_- = N2^N$. Von Neumann's theory ensures that self-adjoint extensions of \hat{H} exist and they are parametrized by the unitary applications between \mathcal{N}_i and \mathcal{N}_{-i} . Accordingly the family of operators which are self-adjoint extensions of \hat{H} is characterized by $(N2^{N+1})^2$ real parameters for $d = 1$ and by $(N2^N)^2$ real parameters for $d = 2, 3$.

Let us denote with $H^{\mathcal{U}}$ the self-adjoint extension of \hat{H} corresponding, via the von Neumann's formula, to the unitary application $\mathcal{U} : \mathcal{N}_i(\hat{H}) \rightarrow \mathcal{N}_{-i}(\hat{H})$. In general, given \mathcal{U} , it is not easy to obtain any information about the resolvent of $H^{\mathcal{U}}$ and the behavior of the wave function component of the generic vector $\Psi \in D(H^{\mathcal{U}})$ in the points y_j .

Since we want to stress the relation between a given self-adjoint operator and the coupling between the wave function and the spin placed in y_j we characterize the self-adjoint extensions in terms of some generalized boundary conditions satisfied by the wave function component of the vector Ψ .

As it is shown in appendix B there is a one to one correspondence between the self-adjoint extensions of a given symmetric operator \hat{H} and the self-adjoint linear relations on \mathbb{C}^m , where $m = n_+(\hat{H}) = n_-(\hat{H})$. We have reported some results ([11]) (see also [68]) where it was showed that, in a very general setting, a generalized Krein's formula for the resolvent exists. Such a formula explicitly gives the resolvent of a self-adjoint extension of a given symmetric operator in terms of the parameters characterizing the boundary conditions satisfied by the vectors in its domain. Moreover the generalized formula for the resolvent avoids the problem of finding the maximal common part of two extensions.

In the following we use these results to obtain a complete characterization in terms of generalized boundary conditions of all the self-adjoint extensions of the operator \hat{H} . Moreover we explicitly give a formula for the resolvent of each self-adjoint extension of \hat{H} .

Let us introduce the following notation. With μ we indicate the multi-index $\mu = (pj\underline{\sigma})$ for $d = 1$ and $\mu = (j\underline{\sigma})$ for $d = 2, 3$. Indices p, p', p'' etc. always assume the values 0 and 1. Indices j, j' and so on run over $1, \dots, N$. With $\underline{\sigma}, \underline{\sigma}'$, etc., we indicate N -dimensional vectors, e.g., $(\sigma_1, \dots, \sigma_N)$ where $\sigma_j = \pm 1$. As an example with this notation the vectors in \mathcal{H} defined by (5.22) and (5.23) are shortly referred to as Φ_μ^z .

In the following $\delta_{i,j}$ indicates the Kronecker symbol

$$\delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \quad (5.25)$$

moreover

$$\delta_{\underline{\sigma}, \underline{\sigma}'} = \delta_{\sigma_1, \sigma'_1} \dots \delta_{\sigma_N, \sigma'_N}. \quad (5.26)$$

Given two $m \times m$ matrices A and B , $(A|B)$ indicates the $m \times 2m$ block matrix with the first m columns given by the columns of A and the second m 's given by the columns of B .

Theorem 5.2.1. ($d = 1$) Define the operator

$$D(H^{AB}) = \left\{ \Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \in \mathcal{H} \mid \psi_{\underline{\sigma}} \in H^2(\mathbb{R} \setminus Y) \forall \underline{\sigma}; \right. \\ \left. \sum_{\mu'} A_{\mu, \mu'} q_{\mu'} = \sum_{\mu'} B_{\mu, \mu'} f_{\mu'}; \right. \quad (5.27)$$

$$q_{0j\underline{\sigma}} = \psi'_{\underline{\sigma}}(y_j^-) - \psi'_{\underline{\sigma}}(y_j^+), \quad q_{1j\underline{\sigma}} = \psi_{\underline{\sigma}}(y_j^-) - \psi_{\underline{\sigma}}(y_j^+), \quad (5.28)$$

$$f_{pj\underline{\sigma}} = (-)^p \frac{\psi_{\underline{\sigma}}^{(p)}(y_j^+) + \psi_{\underline{\sigma}}^{(p)}(y_j^-)}{2}, \quad (5.29)$$

$$AB^* = BA^*, (A|B) \text{ of maximal rank } N2^{N+1} \left. \right\} \quad (5.30)$$

$$H^{AB}\Psi = \sum_{\underline{\sigma}} (-\Delta + \underline{\beta}_{\underline{\sigma}})\psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \quad \beta_j \in \mathbb{R}, x \in \mathbb{R} \setminus Y. \quad (5.31)$$

H^{AB} is self-adjoint and its resolvent, $R^{AB}(z) = (H^{AB} - z)^{-1}$, is given by

$$R^{AB}(z) = R(z) + \sum_{\mu, \mu', \mu''} ((\Gamma^{AB}(z))^{-1})_{\mu, \mu'} B_{\mu', \mu''} \langle \Phi_{\mu''}^{\bar{z}}, \cdot \rangle \Phi_{\mu}^z \quad z \in \rho(H^{AB}). \quad (5.32)$$

Where $\Gamma^{AB}(z)$ is the $N2^{N+1} \times N2^{N+1}$ matrix defined as

$$\Gamma^{AB}(z) = B\Gamma(z) + A. \quad (5.33)$$

with

$$\begin{aligned}
(\Gamma(z))_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= 0 & \underline{\sigma} &\neq \underline{\sigma}' \\
(\Gamma(z))_{pj\underline{\sigma}, p'j'\underline{\sigma}} &= 0 & p &\neq p' \\
(\Gamma(z))_{0j\underline{\sigma}, 0j'\underline{\sigma}} &= -G^{z-\underline{\beta}\underline{\sigma}}(y_j - y_{j'}) \\
(\Gamma(z))_{1j\underline{\sigma}, 1j'\underline{\sigma}} &= -(z - \underline{\beta}\underline{\sigma})G^{z-\underline{\beta}\underline{\sigma}}(y_j - y_{j'}) \\
(\Gamma(z))_{1j\underline{\sigma}, 0j'\underline{\sigma}} &= (G^{z-\underline{\beta}\underline{\sigma}})'(y_j - y_{j'}) & j &\neq j' \\
(\Gamma(z))_{0j\underline{\sigma}, 1j'\underline{\sigma}} &= -(G^{z-\underline{\beta}\underline{\sigma}})'(y_j - y_{j'}) & j &\neq j'.
\end{aligned} \tag{5.34}$$

Functions $G^w(x)$ and $(G^w)'(x)$ are defined in (5.12) and (5.24).

Proof. Define two linear applications $\Lambda : D(\hat{H}^*) \rightarrow \mathbb{C}^m$ and $\tilde{\Lambda} : D(\hat{H}^*) \rightarrow \mathbb{C}^m$, with $m = N2^{N+1}$. Λ defines the charges q_μ in (5.28) by

$$q_\mu = (\Lambda\Psi)_\mu \quad \mu = (pj\underline{\sigma}) ; \quad \Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \in D(\hat{H}^*). \tag{5.35}$$

$\tilde{\Lambda}$ defines f_μ in (5.29)

$$f_\mu = (\tilde{\Lambda}\Psi)_\mu \quad \mu = (pj\underline{\sigma}) ; \quad \Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \in D(\hat{H}^*). \tag{5.36}$$

The linear functionals Λ and $\tilde{\Lambda}$ correspond to Γ_1 and Γ_2 defined in [11]. Integrating by parts it follows that

$$\langle \Psi_1, \hat{H}^*\Psi_2 \rangle - \langle \hat{H}^*\Psi_1, \Psi_2 \rangle = \sum_{\mu} \left[\overline{(\Lambda\Psi_1)_\mu} (\tilde{\Lambda}\Psi_2)_\mu - \overline{(\tilde{\Lambda}\Psi_1)_\mu} (\Lambda\Psi_2)_\mu \right] \tag{5.37}$$

for all $\Psi_1, \Psi_2 \in D(\hat{H}^*)$. Moreover Λ and $\tilde{\Lambda}$ are surjective, this implies that the triple $(\mathbb{C}^m, \Lambda, \tilde{\Lambda})$ is a boundary value space for \hat{H} , see, e.g., [48]. Then from Theorem 3.1.6 in [48] we obtain that all the self-adjoint extensions of \hat{H} correspond to the restrictions of \hat{H}^* on vectors Ψ satisfying

$$\sum_{\mu'} A_{\mu, \mu'} (\Lambda\Psi)_{\mu'} = \sum_{\mu'} B_{\mu, \mu'} (\tilde{\Lambda}\Psi)_{\mu'}, \tag{5.38}$$

where $A_{\mu, \mu'}$ and $B_{\mu, \mu'}$ are two $N2^{N+1}$ matrices satisfying $AB^* = BA^*$ (AB^* Hermitian) and $(A|B)$ with maximal rank $N2^{N+1}$. This proves that the operators H^{AB} are self-adjoint.

We use the proposition proved in [11] (see also Theorem 10 in [68]) to write down the resolvent of H^{AB} .

Define $\gamma_z : \mathbb{C}^m \rightarrow \mathcal{N}_z$ in the following way: $\gamma_z = (\Lambda|\mathcal{N}_z)^{-1}$. The action of γ_z on a vector $\underline{a} \in \mathbb{C}^m$ is given by

$$\gamma_z \underline{a} = \sum_{\mu} a_{\mu} \Phi_{\mu}^z \tag{5.39}$$

where Φ_μ^z is defined in (5.22). In fact

$$(\Lambda \Phi_{p'j'\underline{\sigma}}^z)_{pj\underline{\sigma}} = \delta_{\underline{\sigma}, \underline{\sigma}'} \delta_{j, j'} \delta_{p, p'} [(G^{z-\beta\underline{\sigma}})'(0^-) - (G^{z-\beta\underline{\sigma}})'(0^+)] = \delta_{\underline{\sigma}, \underline{\sigma}'} \delta_{j, j'} \delta_{p, p'}. \quad (5.40)$$

The adjoint of $\gamma_z, \gamma_z^* : \mathcal{H} \rightarrow \mathbb{C}^m$ is defined by

$$(\gamma_z^* \Psi)_\mu = \langle \Phi_\mu^z, \Psi \rangle \quad (5.41)$$

in fact

$$\langle \Psi, \gamma_z \underline{a} \rangle = \sum_{pj\underline{\sigma}} a_{pj\underline{\sigma}} \left(\psi_{\underline{\sigma}}(\cdot), (G^{z-\beta\underline{\sigma}})^{(p)}(\cdot - y_j) \right)_{L^2} = \sum_{pj\underline{\sigma}} \overline{(\gamma_z^* \Psi)_{pj\underline{\sigma}}} a_{pj\underline{\sigma}}. \quad (5.42)$$

By straightforward calculations it is possible to show that the matrix $\Gamma(z) = -\tilde{\Lambda} \gamma_z$ coincides with the definition given in (5.34). From the definition of the domain of H^{AB} it follows that the free Hamiltonian H is the self-adjoint extension of H_0 corresponding to the choice $A = 1$ and $B = 0$. Then γ_z and $\Gamma(z)$ are analytic for $z \in \rho(H)$ and

$$(\Gamma(z))_{\mu, \mu'} - (\Gamma(w))_{\mu, \mu'} = (w - z) \langle \Phi_\mu^{\bar{z}}, \Phi_{\mu'}^w \rangle \quad z, w \in \rho(H). \quad (5.43)$$

Making use of the result stated in [11] (see also Theorem 10 in [68]) we obtain that for all $z \in \rho(H_0) \cap \rho(H^{AB})$ the resolvent formula (5.32) holds. Since the resolvent of H^{AB} is a finite rank perturbation of the resolvent of H we have $\sigma_{ess}(H^{AB}) = \sigma_{ess}(H_0) = \sigma(H_0)$ (see, e.g., [7]), and $\rho(H) \cap \rho(H^{AB}) = \rho(H^{AB})$. \square

Theorem 5.2.2. ($d = 2$)

$$D(H^{AB}) := \left\{ \Psi = \sum_{\sigma} \psi_{\sigma} \otimes \mathcal{X}_{\sigma} \in \mathcal{H} \mid \Psi = \Psi^z + \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z; \Psi^z \in D(H_0); z \in \rho(H^{AB}); \right.$$

$$\left. \sum_{\sigma'} A_{\sigma, \sigma'} q_{\sigma'} = \sum_{\sigma'} B_{\sigma, \sigma'} f_{\sigma'}; \quad (5.44) \right.$$

$$f_{\sigma} = \lim_{|x| \rightarrow 0} \left[\psi_{\sigma}(x) + \frac{q_{\sigma}}{2\pi} \ln(|x|) \right] \quad (5.45)$$

$$AB^* = BA^*, (A|B) \text{ of maximal rank } N2^N \quad (5.46)$$

$$(5.47)$$

$$H^{AB} \Psi := H_0 \Psi^z + z \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z \quad \Psi \in D(H^{AB}). \quad (5.48)$$

H^{AB} is self-adjoint and its resolvent, $R^{AB}(z) = (H^{AB} - z)^{-1}$, is given by

$$R^{AB}(z) = R(z) + \sum_{\sigma, \sigma', \sigma''} ((\Gamma^{AB}(z))^{-1})_{\sigma, \sigma'} B_{\sigma', \sigma''} \langle \Phi_{\sigma''}^{\bar{z}}, \cdot \rangle \Phi_{\sigma}^z \quad z \in \rho(H^{AB}). \quad (5.49)$$

Where $\Gamma^{AB}(z)$ is the $N2^N \times N2^N$ matrix

$$\Gamma^{AB}(z) = B\Gamma(z) + A, \quad (5.50)$$

with

$$\begin{aligned}
(\Gamma(z))_{j\underline{\sigma},j'\underline{\sigma}'} &= 0 & \underline{\sigma} &\neq \underline{\sigma}' \\
(\Gamma(z))_{j\underline{\sigma},j\underline{\sigma}} &= \frac{\ln(\sqrt{z - \sigma\beta/2}) + \gamma - i\pi/2}{2\pi} \\
(\Gamma(z))_{j\underline{\sigma},j'\underline{\sigma}} &= -G^{z-\beta\underline{\sigma}}(y_j - y_{j'}) & j &\neq j'.
\end{aligned} \tag{5.51}$$

Proof. Let us give a sketch of the proof, it strictly follows the proof of theorem 5.2.1

Define two linear applications $\Lambda : D(S^*) \rightarrow \mathbb{C}^2$ and $\tilde{\Lambda} : D(S^*) \rightarrow \mathbb{C}^2$, Λ defines the coefficient of singularity (the charge) of wave function part of vectors in $D(S^*)$,

$$(\Lambda\Psi)_\sigma = q_\sigma = - \lim_{|x| \rightarrow 0} \frac{2\pi}{\ln(|x|)} \psi_\sigma(x) \quad \Psi = \sum_\sigma \psi_\sigma \otimes \chi_\sigma \in D(S^*) \tag{5.52}$$

$\tilde{\Lambda}$ defines the value in the origin of regular part of wave function, f_σ ,

$$f_\sigma = (\tilde{\Lambda}\Psi)_\sigma \quad \Psi = \sum_\sigma \psi_\sigma \otimes \chi_\sigma \in D(S^*). \tag{5.53}$$

A direct calculation shows that the triple $(\mathbb{C}^m, \Lambda, \tilde{\Lambda})$ is a boundary value space for S (see, e.g., Appendix B, [48]), i.e. for all $\Psi_1, \Psi_2 \in D(S^*)$

$$\langle \Psi_1, S^*\Psi_2 \rangle - \langle S^*\Psi_1, \Psi_2 \rangle = \sum_\sigma \left[\overline{(\Lambda\Psi_1)_\sigma} (\tilde{\Lambda}\Psi_2)_\sigma - \overline{(\tilde{\Lambda}\Psi_1)_\sigma} (\Lambda\Psi_2)_\sigma \right] \tag{5.54}$$

and Λ and $\tilde{\Lambda}$ are surjective. Then all self-adjoint extensions of S are given by restrictions of S^* on vectors Ψ satisfying

$$\sum_{\sigma'} A_{\sigma,\sigma'} (\Lambda\Psi)_{\sigma'} = \sum_{\sigma'} B_{\sigma,\sigma'} (\tilde{\Lambda}\Psi)_{\sigma'}, \tag{5.55}$$

where A and B are two 2×2 matrices satisfying $AB^* = BA^*$ and $(A|B)$ with maximal rank (see e.g. Theorem 3.1.6 in [48]). This proves that operators H^{AB} are self-adjoint.

Resolvent of H^{AB} comes directly from resolvent formula in [11] (see also Theorem 10 in [68]). \square

An analogous theorem holds in the three dimensional case.

Theorem 5.2.3. ($d = 3$) Define the operator

$$D(H^{AB}) = \left\{ \Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \in \mathcal{H} \mid \Psi = \Psi^z + \sum_{\mu} q_{\mu} \Phi_{\mu}^z; \right. \\ \Psi^z \in D(H_0); z \in \rho(H^{AB}); \\ \left. \sum_{\mu'} A_{\mu, \mu'} q_{\mu'} = \sum_{\mu'} B_{\mu, \mu'} f_{\mu'}; \right. \quad (5.56)$$

$$q_{j\underline{\sigma}} = \lim_{|x-y_j| \rightarrow 0} 4\pi |x-y_j| \psi_{\underline{\sigma}}(x), \quad (5.57)$$

$$f_{j\underline{\sigma}} = \lim_{|x-y_j| \rightarrow 0} \left[\psi_{\underline{\sigma}}(x) - \frac{q_{j\underline{\sigma}}}{4\pi |x-y_j|} \right], \quad (5.58)$$

$$AB^* = BA^*, (A|B) \text{ of maximal rank } N2^N \} \quad (5.59)$$

$$H^{AB}\Psi = H_0\Psi^z + z \sum_{j, \underline{\sigma}} q_{j\underline{\sigma}} \Phi_{j\underline{\sigma}}^z \quad \Psi \in D(H^{AB}). \quad (5.60)$$

H^{AB} is self-adjoint and its resolvent, $R^{AB}(z) = (H^{AB} - z)^{-1}$, is given by

$$R^{AB}(z) = R(z) + \sum_{\mu, \mu', \mu''} ((\Gamma^{AB}(z))^{-1})_{\mu, \mu'} B_{\mu', \mu''} \langle \Phi_{\mu''}^z, \cdot \rangle \Phi_{\mu}^z \quad z \in \rho(H^{AB}). \quad (5.61)$$

Where $\Gamma^{AB}(z)$ is the $N2^N \times N2^N$ matrix defined as

$$\Gamma^{AB}(z) = B\Gamma(z) + A. \quad (5.62)$$

with

$$(\Gamma(z))_{j\underline{\sigma}, j'\underline{\sigma}'} = 0 \quad \underline{\sigma} \neq \underline{\sigma}' \\ (\Gamma(z))_{j\underline{\sigma}, j\underline{\sigma}} = \frac{\sqrt{z - \beta \underline{\sigma}}}{4\pi i} \\ (\Gamma(z))_{j\underline{\sigma}, j'\underline{\sigma}} = -G^{z - \beta \underline{\sigma}}(y_j - y_{j'}) \quad j \neq j'. \quad (5.63)$$

Function $G^w(x)$ is defined in (5.12).

Proof. The proof of the self-adjointness of H^{AB} is basically the same as in the one dimensional case. Two linear, surjective applications $\Lambda, \tilde{\Lambda} : D(\hat{H}^*) \rightarrow \mathbb{C}^m$ define the charges $q_{j\underline{\sigma}}$ and the values $f_{j\underline{\sigma}}$ as it was done in the one dimensional case, see (5.35) and (5.36). The von Neumann decomposition formula (see, e.g., [76]) gives the following expression for the generic vector in $D(\hat{H}^*)$

$$\Psi = \Psi_0 + \sum_{\mu} (a_{\mu} \Phi_{\mu}^i + b_{\mu} \Phi_{\mu}^{-i}) \quad a_{\mu}, b_{\mu} \in \mathbb{C}; \Psi_0 \in D(\hat{H}) \quad (5.64)$$

with $\Phi_{\mu}^{\pm i}$ as in (5.23). The action of \hat{H}^* on its domain can be written as

$$\hat{H}^*\Psi = \hat{H}\Psi_0 + i \sum_{\mu} (a_{\mu} \Phi_{\mu}^i - b_{\mu} \Phi_{\mu}^{-i}) \quad a_{\mu}, b_{\mu} \in \mathbb{C}; \Psi_0 \in D(\hat{H}). \quad (5.65)$$

By using the symmetry of \hat{H} it is easily proved that, given $\Psi_1, \Psi_2 \in D(\hat{H}^*)$ such that

$$\Psi_k = \Psi_{k,0} + \sum_{\mu} (a_{k,\mu} \Phi_{\mu}^i + b_{k,\mu} \Phi_{\mu}^{-i}) \quad a_{k,\mu}, b_{k,\mu} \in \mathbb{C}; \Psi_{k,0} \in D(\hat{H}), k = 1, 2 \quad (5.66)$$

the following relation holds

$$\begin{aligned} & \langle \Psi_1, \hat{H}^* \Psi_2 \rangle - \langle \hat{H}^* \Psi_1, \Psi_2 \rangle = \\ & = 2i \sum_{j,j',\underline{\sigma}} (\bar{a}_{1,j\underline{\sigma}} a_{2,j'\underline{\sigma}} - \bar{b}_{1,j\underline{\sigma}} b_{2,j'\underline{\sigma}}) (G^{i-\underline{\beta}\underline{\sigma}}(\cdot - y_j), G^{i-\underline{\beta}\underline{\sigma}}(\cdot - y_{j'}))_{L^2}. \end{aligned} \quad (5.67)$$

On the other hand,

$$(\Lambda \Psi_k)_{\mu} = q_{k,\mu} = a_{k,\mu} + b_{k,\mu} \quad k = 1, 2 \quad (5.68)$$

and

$$\begin{aligned} (\tilde{\Lambda} \Psi_k)_{j\underline{\sigma}} = f_{k,j\underline{\sigma}} = & i \left(a_{k,j\underline{\sigma}} \frac{\sqrt{i - \underline{\beta}\underline{\sigma}}}{4\pi} + b_{k,j\underline{\sigma}} \frac{\sqrt{-i - \underline{\beta}\underline{\sigma}}}{4\pi} \right) + \\ & + \sum_{j' \neq j} \left(a_{k,j'\underline{\sigma}} G^{i-\underline{\beta}\underline{\sigma}}(y_j - y_{j'}) + b_{k,j'\underline{\sigma}} G^{-i-\underline{\beta}\underline{\sigma}}(y_j - y_{j'}) \right) \quad k = 1, 2. \end{aligned} \quad (5.69)$$

The right hand side of relation (5.37) then reads

$$\begin{aligned} & \sum_{\mu} \left[\overline{(\Lambda \Psi_1)_{\mu}} (\tilde{\Lambda} \Psi_2)_{\mu} - \overline{(\tilde{\Lambda} \Psi_1)_{\mu}} (\Lambda \Psi_2)_{\mu} \right] = \\ & = \frac{i}{4\pi} (\bar{a}_{1,j\underline{\sigma}} a_{2,j\underline{\sigma}} - \bar{b}_{1,j\underline{\sigma}} b_{2,j\underline{\sigma}}) (\sqrt{i - \underline{\beta}\underline{\sigma}} - \sqrt{-i - \underline{\beta}\underline{\sigma}}) + \\ & + \sum_{j' \neq j} (\bar{a}_{1,j\underline{\sigma}} a_{2,j'\underline{\sigma}} - \bar{b}_{1,j\underline{\sigma}} b_{2,j'\underline{\sigma}}) (G^{i-\underline{\beta}\underline{\sigma}}(y_j - y_{j'}) - G^{-i-\underline{\beta}\underline{\sigma}}(y_j - y_{j'})). \end{aligned} \quad (5.70)$$

By using the resolvent identity on $(G^{i-\underline{\beta}\underline{\sigma}}(\cdot - y_j), G^{i-\underline{\beta}\underline{\sigma}}(\cdot - y_{j'}))_{L^2}$, for $j \neq j'$, and by direct computation of $\|G^{i-\underline{\beta}\underline{\sigma}}\|_{L^2}^2$ it is shown that (5.67) and (5.70) coincide. Then, also for $d = 3$, the triple $(\mathbb{C}^m, \Lambda, \tilde{\Lambda})$ is a boundary value space and the restriction of \hat{H}^* to vectors satisfying (5.56) is self-adjoint, we indicate such a restriction with \tilde{H}^{AB} . Assume that $\Psi \in \tilde{H}^{AB}$ and that it is written as in formula (5.64), posing

$$\Psi = \Psi^z + \sum_{\mu} q_{\mu} \Phi_{\mu}^z \quad (5.71)$$

with

$$\Psi^z = \Psi_0 + \sum_{\mu} (a_{\mu} \Phi_{\mu}^i + b_{\mu} \Phi_{\mu}^{-i} - q_{\mu} \Phi_{\mu}^z), \quad (5.72)$$

and noticing that $q_\mu = a_\mu + b_\mu$, it follows that $\Psi^z \in D(H_0)$ and that the action of \tilde{H}^{AB} on its domain is given by (5.60). Then H^{AB} is self-adjoint.

Define $\gamma_z : \mathbb{C}^m \rightarrow \mathcal{N}_z$ as before: $\gamma_z = (\Lambda|\mathcal{N}_z)^{-1}$. Analogously to the one dimensional case, given a vector $\underline{a} \in \mathbb{C}^m$, $\gamma_z \underline{a} = \sum_\mu a_\mu \Phi_\mu^z$ (see Theorem 5.2.1). Its adjoint is $\gamma_z^* : \mathcal{H} \rightarrow \mathbb{C}^m$, $(\gamma_z^* \Psi)_\mu = \langle \Phi_\mu^z, \Psi \rangle$. As in the one dimensional case it is possible to show that the matrix $\Gamma(z) = -\tilde{\Lambda} \gamma_z$ coincides with the definition given in (5.63). The free Hamiltonian H corresponds to the choice $A = 1$ and $B = 0$, and the resolvent formula (5.61) follows as in the one dimensional case. \square

If the matrix B is invertible the generalized Krein formula is easily reduced to the standard formula with one matrix usually denoted with Θ , see [73].

The generalized boundary conditions of the form (5.27) and (5.56) include both local and non local interactions. In our setting local means that the behavior of the wave function in the point y_j depends only on the state of the spin placed in the point y_j . The sub-family of local Hamiltonians H^{AB} , the only ones generally considered physically admissible, is obtained by imposing some restrictions on the matrices A and B , i.e.

$$d = 1$$

$$\begin{aligned} A_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= B_{pj\underline{\sigma}, p'j'\underline{\sigma}'} = 0 & \forall j \neq j' \\ A_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= B_{pj\underline{\sigma}, p'j'\underline{\sigma}'} = 0 & \text{if for some } k \neq j, \sigma_k \neq \sigma'_k \\ A_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= a_{pj\underline{\sigma}, p'j'\underline{\sigma}'}; & B_{pj\underline{\sigma}, p'j'\underline{\sigma}'} = b_{pj\underline{\sigma}, p'j'\underline{\sigma}'} \quad \text{otherwise} \end{aligned} \quad (5.73)$$

$$d = 2, 3$$

$$\begin{aligned} A_{j\underline{\sigma}, j'\underline{\sigma}'} &= B_{j\underline{\sigma}, j'\underline{\sigma}'} = 0 & \forall j \neq j' \\ A_{j\underline{\sigma}, j'\underline{\sigma}'} &= B_{j\underline{\sigma}, j'\underline{\sigma}'} = 0 & \text{if for some } k \neq j, \sigma_k \neq \sigma'_k \\ A_{j\underline{\sigma}, j'\underline{\sigma}'} &= a_{j\underline{\sigma}, j'\underline{\sigma}'}; & B_{j\underline{\sigma}, j'\underline{\sigma}'} = b_{j\underline{\sigma}, j'\underline{\sigma}'} \quad \text{otherwise} \end{aligned} \quad (5.74)$$

where the (complex) constants $a_{pj\underline{\sigma}, p'j'\underline{\sigma}'}$, $b_{pj\underline{\sigma}, p'j'\underline{\sigma}'}$ (and $a_{j\underline{\sigma}, j'\underline{\sigma}'}$, $b_{j\underline{\sigma}, j'\underline{\sigma}'}$) are subjected to the restriction (5.30) (and (5.59)).

We give the explicit form of two local Hamiltonians that we consider of special interest.

Example 5.2.1. *δ -like interactions.*

Consider the following choice for the matrices A and B

$$d = 1$$

$$\begin{aligned} a_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= \delta_{p,p'} \delta_{\sigma_j, \sigma'_j} \\ b_{0j\underline{\sigma}, 0j'\underline{\sigma}'} &= -2\alpha_{j\underline{\sigma}} \delta_{\sigma_j, \sigma'_j} \\ b_{pj\underline{\sigma}, p'j'\underline{\sigma}'} &= 0 \quad \text{for } p \neq 0 \text{ or } p' \neq 0 \\ &\text{with } \alpha_{j\underline{\sigma}} \in \mathbb{R} \end{aligned}$$

$$d = 2, 3$$

$$\begin{aligned} a_{j\underline{\sigma}, j'\underline{\sigma}'} &= \alpha_{j\underline{\sigma}} \delta_{\sigma_j, \sigma'_j} \\ b_{j\underline{\sigma}, j'\underline{\sigma}'} &= \delta_{\sigma_j, \sigma'_j} \\ &\text{with } \alpha_{j\underline{\sigma}} \in \mathbb{R} \end{aligned} \quad (5.75)$$

We indicate with H^δ the generic Hamiltonian in this sub-family of local interactions. For $d = 1$, the wave function component of the generic state $\Psi \in D(H^\delta)$ is continuous but with discontinuous derivative, in particular the following boundary conditions hold

$$\psi_{\underline{\sigma}}(y_j^+) = \psi_{\underline{\sigma}}(y_j^-) \equiv \psi_{\underline{\sigma}}(y_j), \quad \psi'_{\underline{\sigma}}(y_j^+) - \psi'_{\underline{\sigma}}(y_j^-) = \alpha_{j\sigma_j} \psi_{\underline{\sigma}}(y_j). \quad (5.76)$$

For $d = 2, 3$ the boundary conditions simply read

$$\alpha_{j\sigma_j} q_{j\underline{\sigma}} = f_{j\underline{\sigma}}. \quad (5.77)$$

Comparing the Hamiltonians we define in the one particle case in chapter 3 it is clear that the H^δ are point interaction Hamiltonians with spin dependent strength. We would like to stress that such boundary conditions are diagonal in the spin variables. This means that the χ_+ component of the j -th spin affects only the wave function component relative to the configuration of the spins with the j -th one in the state χ_+ . This implies that, given the initial state $\Psi^{t=0} = \psi^0 \otimes \mathcal{X}_{\underline{\sigma}}$, the evolution generated by H^δ gives $\Psi^t = \psi^t \otimes \mathcal{X}_{\underline{\sigma}}$. Here $\psi^t(x) = (U_\beta^t \psi^0)(x)$, where U_β^t is a strongly continuous unitary group in $L^2(\mathbb{R}^d)$.

Example 5.2.2. *Off diagonal interactions.*

Let us consider the local interactions defined by

$$\begin{aligned} d = 1 & & d = 2, 3 \\ a_{pj\sigma_j, p'j\sigma'_j} &= \delta_{p,p'} \delta_{\sigma_j, \sigma'_j} & a_{j\sigma_j, j\sigma'_j} &= \sigma_j i \hat{\alpha}_{j\sigma_j} (1 - \delta_{\sigma_j, \sigma'_j}) \\ b_{0j\sigma_j, 0j\sigma'_j} &= -2\sigma_j i \hat{\alpha}_{j\sigma_j} (1 - \delta_{\sigma_j, \sigma'_j}) & b_{j\sigma_j, j\sigma'_j} &= \delta_{\sigma_j, \sigma'_j} \\ b_{pj\sigma_j, p'j\sigma'_j} &= 0 \quad \text{for } p \neq 0 \text{ or } p' \neq 0 & & \text{with } \hat{\alpha}_{j\sigma_j} \in \mathbb{R} \\ & & & \text{with } \hat{\alpha}_{j\sigma_j} \in \mathbb{R} \end{aligned} \quad (5.78)$$

A simple calculation gives the corresponding boundary conditions. For $d = 1$

$$\begin{aligned} \psi_{\underline{\sigma}}(y_j^+) &= \psi_{\underline{\sigma}}(y_j^-) \equiv \psi_{\underline{\sigma}}(y_j) \\ \psi'_{\underline{\sigma}}(y_j^+) - \psi'_{\underline{\sigma}}(y_j^-) &= \sigma_j i \alpha_{j\sigma_j} \psi_{(\sigma_1 \dots \sigma'_j \dots \sigma_N)}(y_j) \quad \sigma'_j \neq \sigma_j. \end{aligned} \quad (5.79)$$

and for $d = 3$

$$\sigma_j i \hat{\alpha}_{j\sigma_j} q_{j(\sigma_1 \dots \sigma'_j \dots \sigma_N)} = f_{j\underline{\sigma}} \quad \sigma'_j \neq \sigma_j. \quad (5.80)$$

The class of Hamiltonians proposed in this second example are the simplest off diagonal ones. The interaction with the particle induces the spins to evolve towards a superposition state also when the initial state is such that every spin is in an eigenstate of $\hat{\sigma}_j^{(1)}$, $\Psi^{t=0} = \psi^0 \otimes \mathcal{X}_{\underline{\sigma}}$.

We regard as useful to give, at least in the simplest case of one spin, the explicit expression of the resolvent of the Hamiltonians proposed in examples 5.2.1 and 5.2.2. This is done in the following:

Example 5.2.3. *One spin in dimension three.*

Let us consider the case of one spin in dimension three placed in the point $y \in \mathbb{R}^3$. We indicate with $R^\delta(z)$ the resolvent of the Hamiltonian H^δ defined in example 5.2.1 when $N = 1$. The resolvent $R^\delta(z)$ can be written as

$$\begin{aligned} R^\delta(z) = & \left[G^{z-\beta} + \frac{4\pi i}{\sqrt{z-\eta} + 4\pi i \alpha_+} G^{z-\beta}(\cdot - y) G^{z-\beta}(y - \cdot) \right] \otimes (\chi_+, \cdot)_{\mathbb{C}^2} \chi_{++} \\ & + \left[G^{z+\beta} + \frac{4\pi i}{\sqrt{z+\beta} + 4\pi i \alpha_-} G^{z+\beta}(\cdot - y) G^{z+\beta}(y - \cdot) \right] \otimes (\chi_-, \cdot)_{\mathbb{C}^2} \chi_{--}. \end{aligned} \quad (5.81)$$

The expressions in the square brackets are identical to the resolvent of the operator formally written as “ $-\Delta + \beta_\sigma \delta_y$ ” in dimension three (see [9]). Then all the results concerning the delta-potential in dimension three can be adapted to H^δ . Let us recall that the generator of the dynamics can be formally written as $e^{-iH^\delta t} = -\mathcal{L}^{-1}((H^\delta - \cdot)^{-1})(-it)$, then, due to the presence of the projectors $(\chi_+, \cdot)_{\mathbb{C}^2} \chi_{++}$ and $(\chi_-, \cdot)_{\mathbb{C}^2} \chi_{--}$ the dynamics generated by H^δ is factorized in the spin components.

Let us indicate with H^{od} the Hamiltonian corresponding to the one defined in example 5.2.2, in dimension three and with $N = 1$. Its resolvent can be explicitly written with the following large formula

$$\begin{aligned} R^{od}(z) = & G^{z-\beta} \otimes (\chi_+, \cdot)_{\mathbb{C}^2} \chi_{++} + G^{z+\beta} \otimes (\chi_-, \cdot)_{\mathbb{C}^2} \chi_{--} \\ & - \frac{4\pi i \sqrt{z+\beta}}{(4\pi)^2 \hat{\alpha}_+ \hat{\alpha}_- - \sqrt{z-\beta} \sqrt{z+\beta}} G^{z-\beta}(\cdot - y) G^{z-\beta}(y - \cdot) \otimes (\chi_+, \cdot)_{\mathbb{C}^2} \chi_{++} \\ & - \frac{4\pi i \sqrt{z-\beta}}{(4\pi)^2 \hat{\alpha}_+ \hat{\alpha}_- - \sqrt{z-\beta} \sqrt{z+\beta}} G^{z+\beta}(\cdot - y) G^{z+\beta}(y - \cdot) \otimes (\chi_-, \cdot)_{\mathbb{C}^2} \chi_{--} \quad (5.82) \\ & - \frac{i \hat{\alpha}_+}{(4\pi)^2 \hat{\alpha}_+ \hat{\alpha}_- - \sqrt{z-\beta} \sqrt{z+\beta}} G^{z-\beta}(\cdot - y) G^{z+\beta}(y - \cdot) \otimes (\chi_-, \cdot)_{\mathbb{C}^2} \chi_{++} \\ & + \frac{i \hat{\alpha}_-}{(4\pi)^2 \hat{\alpha}_+ \hat{\alpha}_- - \sqrt{z-\beta} \sqrt{z+\beta}} G^{z+\beta}(\cdot - y) G^{z-\beta}(y - \cdot) \otimes (\chi_+, \cdot)_{\mathbb{C}^2} \chi_{--} \end{aligned}$$

The terms $(\chi_-, \cdot)_{\mathbb{C}^2} \chi_{++}$ and $(\chi_+, \cdot)_{\mathbb{C}^2} \chi_{--}$ indicate that, in such a case, the dynamics cannot be factorized in the spin components. Furthermore there are not “ready to use” formulas that can be used to evaluate the spectrum or the propagator of H^{od} .

Chapter 6

A model for a tracking chamber

Introduction

In the previous chapter we introduced a family of Hamiltonians describing the dynamics of a quantum system consisting of one particle in interaction with an array of localized spins.

We have found and made explicit different self-adjoint extensions of the free Hamiltonian corresponding to different physical models of interaction between the particle and the spins. We have seen that is possible to characterize particular subfamilies of extensions according to different features of the dynamics they generate, in particular we identified the sub-family of δ -like Hamiltonians. In this case the spin dynamics is unaffected by the interaction, the particle “feels” zero-range forces whose strength depends on the value of some spin component of the localized spin.

In this chapter our aim is to build up simple models for a quantum measurement apparatus detecting “the trajectory” of a quantum particle. In a seminal paper [66] Sir Neville Mott was looking for an explanation of the appearance of sharp classical-like tracks in particle detectors in high energy Physics experiments. Mott’s paper remained almost unnoticed till the second half of the last century when a renewed interest in the measurement problem showed up in the community of theoretical physicists. Since that time the possibility to understand at least some qualitative features of the measurement process thoroughly inside the framework of Quantum Mechanics, without relying on any “reduction of the wave packet” postulate, has been matter of debate in fundamental and applied Theoretical Physics (see, e.g., [52], [57], [38], [5], [4], [27]). We present in this chapter a model of a tracking chamber in which the detectors are represented by spins placed in fixed positions of space and the interaction between the particle and the spins is modelled by a zero range potential. The Hamiltonian is chosen among the ones characterized in the previous chapter for the three dimensional case. The knowledge of the resolvent and of the

spectrum allows to avoid perturbation theory.

In the same spirit of Mott's paper we consider the easiest case where the model tracking chamber is made of only two spins. We prove that given an initial state with the particle described by an outgoing spherical wave function centered in the origin and the spins both in the state down, the probability to find the spins both in the state up as t goes to infinity has a maximum when the positions of the spins are aligned with the origin.

6.1 The model

The system under analysis consists of one quantum particle in \mathbb{R}^3 and two spins 1/2 placed in fixed positions of space, we indicate with $y_1, y_2 \in \mathbb{R}^3$ the positions of the two spins.

Our system will be described in the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \otimes \mathbb{C}^2. \quad (6.1)$$

According to the results of last chapter rephrased in the case of a two spin system, we indicate with a capital Greek letter a vector in \mathcal{H} ; given $\Psi \in \mathcal{H}$ the following decomposition formula holds

$$\Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}}, \quad (6.2)$$

where $\underline{\sigma}$ indicates the two-components vector $\underline{\sigma} = (\sigma_1, \sigma_2)$ with $\sigma_1, \sigma_2 = \pm$ and the sum runs over all the possible choices of σ_1 and σ_2 . The vector $\mathcal{X}_{\underline{\sigma}}$ in $\mathbb{C}^2 \otimes \mathbb{C}^2$ is defined by

$$\mathcal{X}_{\underline{\sigma}} = \chi_{\sigma_1} \otimes \chi_{\sigma_2} \quad (6.3)$$

In our model of a tracking chamber the spins are detectors for the position of the particle. For this reason, among all the Hamiltonians that are point perturbations of H we chose the simplest ones generating a dynamics such that the two spins change their states as a consequence of the interaction with the particle, that is the ones described in section 5.2.2.

Now we give the characterization of the Hamiltonian: the domain of H_α and its action clarifies some details of the interaction between the particle and the

spins

$$\begin{aligned}
D(H_\alpha) = & \left\{ \Psi = \sum_{\underline{\sigma}} \psi_{\underline{\sigma}} \otimes \mathcal{X}_{\underline{\sigma}} \in \mathcal{H} : \Psi = \Psi^z + \sum_{j, \underline{\sigma}} q_{j\underline{\sigma}} \frac{e^{i\sqrt{z-\underline{\beta}\underline{\sigma}}|\cdot-y_j|}}{4\pi|\cdot-y_j|} \otimes \mathcal{X}_{\underline{\sigma}}; \right. \\
& \Psi^z \in D(H_0), \quad z \in \rho(H_\alpha), \quad \Im \sqrt{z-\underline{\beta}\underline{\sigma}} > 0, \quad q_{j\underline{\sigma}} \in \mathbb{C}, \\
& \lim_{|x-y_1| \rightarrow 0} \left(\psi_{(\pm, \sigma_2)}(x) - \frac{q_{1(\pm, \sigma_2)}}{4\pi|x-y_1|} \right) = \pm i\alpha q_{1(\mp, \sigma_2)} \\
& \left. \lim_{|x-y_2| \rightarrow 0} \left(\psi_{(\sigma_1, \pm)}(x) - \frac{q_{2(\sigma_1, \pm)}}{4\pi|x-y_2|} \right) = \pm i\alpha q_{2(\sigma_1, \mp)} \right\}
\end{aligned} \tag{6.4}$$

$$H_\alpha \Psi = H_0 \Psi^z + z \sum_{j, \underline{\sigma}} q_{j\underline{\sigma}} \frac{e^{i\sqrt{z-\underline{\beta}\underline{\sigma}}|\cdot-y_j|}}{4\pi|\cdot-y_j|} \otimes \mathcal{X}_{\underline{\sigma}}; \quad \Psi \in D(\hat{H}). \tag{6.5}$$

Following the standard terminology used for the point perturbations of the Laplacian we refer to the constants $q_{j\underline{\sigma}}$ as charges. Notice that

$$q_{j\underline{\sigma}} = \lim_{|x-y_j| \rightarrow 0} 4\pi|x-y_j|\psi_{\underline{\sigma}}(x) = \sum_{j', \underline{\sigma}'} (\Gamma_\alpha(z))_{j\underline{\sigma}, j'\underline{\sigma}'}^{-1} \psi_{\underline{\sigma}'}^z(y_{j'}) \tag{6.6}$$

then $q_{j\underline{\sigma}}$ is related to the coefficient of the singular term in the point y_j of the wave function part of the state Ψ relative to the configuration of the spins defined by $\underline{\sigma}$.

6.2 Scattering theory

To analyze the state of the system when t goes to infinity we will make use of scattering theory. In this section we introduce some notation and we state the main results about scattering theory for the pair of Hamiltonians H_α and H_0 . Since H_0 and H_α are two different self-adjoint extensions of the same symmetric operator with finite deficiency indices, the wave operators

$$W_\pm = \text{s-} \lim_{t \rightarrow \pm\infty} e^{iH_\alpha t} e^{-iH_0 t} \tag{6.7}$$

exist and are complete (see, e.g., Lemma 4.2.1 in [7]).

Proposition 1. *Assume that $(|y_1 - y_2|\alpha)^{-1} \ll 1$ and $\alpha^2 \gg \beta$ then there are no eigenvalues embedded in the continuous spectrum.*

Proof. By a direct calculation one can show that

$$\text{Det} \left[\Gamma_\alpha(z) \right] = \left(\alpha^2 + \frac{\sqrt{z}\sqrt{z+2\beta}}{(4\pi)^2} \right)^2 \left(\alpha^2 + \frac{\sqrt{z}\sqrt{z-2\beta}}{(4\pi)^2} \right)^2 + O((|y_1 - y_2|\alpha)^{-2}). \tag{6.8}$$

Then the following series expansions hold for the eigenvalues, λ_1 and λ_2 , of H_α

$$\begin{aligned}\lambda_1 &= \beta - \sqrt{\beta^2 + (4\pi\alpha)^4} + O((|y_1 - y_2|\alpha)^{-2}) \\ \lambda_2 &= -\beta - \sqrt{\beta^2 + (4\pi\alpha)^4} + O((|y_1 - y_2|\alpha)^{-2}),\end{aligned}\tag{6.9}$$

for $\alpha^2 \gg \beta$ both λ_1 and λ_2 are less than -2β . \square

In the following we will assume that the hypothesis of proposition 1 are satisfied, in this way we will avoid the occurrence of eigenvalues embedded in the continuous spectrum for the Hamiltonian H_α .

With $L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega)$ we indicate the Hilbert space with scalar product

$$(\psi_1, \psi_2)_{L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega)} = \int_{\underline{\sigma}\underline{\beta}}^{\infty} d\lambda \int_{\Omega} d\omega \overline{\psi_1}(\lambda, \omega) \psi_2(\lambda, \omega)\tag{6.10}$$

where Ω is the solid angle.

Define the map

$$\mathcal{F}_\alpha : \mathcal{H} \rightarrow \bigoplus_{\underline{\sigma}} L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega)\tag{6.11}$$

$$\mathcal{F}_\alpha \Psi := \bigoplus_{\underline{\sigma}} \langle \Phi_\alpha^\sigma, \Psi \rangle = \bigoplus_{\underline{\sigma}} \tilde{\psi}_\alpha^\sigma\tag{6.12}$$

where

$$\begin{aligned}\Phi_\alpha^\sigma(\lambda, \omega) &= \frac{(\lambda - \underline{\beta}\underline{\sigma})^{\frac{1}{4}}}{4\pi^{\frac{3}{2}}} \left[e^{i\sqrt{\lambda - \underline{\beta}\underline{\sigma}}\omega} \otimes \mathcal{X}_{\underline{\sigma}} + \right. \\ &\quad \left. + \sum_{j', \underline{\sigma}', j} (\Gamma_\alpha(\lambda))_{j', \underline{\sigma}', j}^{-1} e^{i\sqrt{\lambda - \underline{\beta}\underline{\sigma}}\omega y_j} \frac{e^{-i\sqrt{\lambda - \underline{\beta}\underline{\sigma}'}\cdot -y_{j'}}}{4\pi|\cdot -y_{j'}} \otimes \mathcal{X}_{\underline{\sigma}'} \right]; \quad \lambda \geq \underline{\sigma}\underline{\beta}, \lambda \geq \underline{\sigma}'\underline{\beta},\end{aligned}\tag{6.13}$$

and

$$\begin{aligned}\Phi_\alpha^\sigma(\lambda, \omega) &= \frac{(\lambda - \underline{\beta}\underline{\sigma})^{\frac{1}{4}}}{4\pi^{\frac{3}{2}}} \left[e^{i\sqrt{\lambda - \underline{\beta}\underline{\sigma}}\omega} \otimes \mathcal{X}_{\underline{\sigma}} + \right. \\ &\quad \left. + \sum_{j', \underline{\sigma}', j} (\Gamma_\alpha(\lambda))_{j', \underline{\sigma}', j}^{-1} e^{i\sqrt{\lambda - \underline{\beta}\underline{\sigma}}\omega y_j} \frac{e^{-\sqrt{\underline{\beta}\underline{\sigma}' - \lambda}\cdot -y_{j'}}}{4\pi|\cdot -y_{j'}} \otimes \mathcal{X}_{\underline{\sigma}'} \right]; \quad \lambda \geq \underline{\sigma}\underline{\beta}, \lambda \leq \underline{\sigma}'\underline{\beta},\end{aligned}\tag{6.14}$$

with

$$(\Gamma_\alpha(\lambda))_{j', \underline{\sigma}', j} = \lim_{\varepsilon \rightarrow 0^+} (\Gamma_\alpha(\lambda - i\varepsilon))_{j', \underline{\sigma}', j}.\tag{6.15}$$

Under the assumptions of proposition 1 the essential spectrum of H_α is only absolutely continuous and coincides with $[\underline{\beta}\underline{\sigma}, +\infty)$. We denote by $P_{\sigma_{ac}(H_\alpha)}$ the

projector on the continuous part of the spectrum of H_α . The map \mathcal{F}_α is unitary on $\mathcal{H}_{ac}(H_\alpha)$, where $\mathcal{H}_{ac}(H_\alpha) = P_{\sigma_{ac}(H_\alpha)}\mathcal{H}$, and its inverse is

$$\mathcal{F}_\alpha^{-1} : \bigoplus_{\underline{\sigma}} L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega) \rightarrow \mathcal{H}_{ac}(H_\alpha) \quad (6.16)$$

$$\mathcal{F}_\alpha^{-1} \bigoplus_{\underline{\sigma}} \tilde{\psi}_\alpha^\sigma = \sum_{\underline{\sigma}} \int_{\underline{\sigma}\underline{\beta}}^{\infty} d\lambda \int_{\Omega} d\omega \Phi_\alpha^\sigma(\lambda, \omega) \tilde{\psi}_\alpha^\sigma(\lambda, \omega). \quad (6.17)$$

Define the map $\mathcal{F} : \mathcal{H} \rightarrow \bigoplus_{\underline{\sigma}} L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega)$

$$\mathcal{F}\Psi := \bigoplus_{\underline{\sigma}} \langle \Phi^\sigma, \Psi \rangle = \bigoplus_{\underline{\sigma}} \tilde{\psi}^\sigma \quad (6.18)$$

where

$$\Phi^\sigma(\lambda, \omega) = \frac{(\lambda - \underline{\beta}\underline{\sigma})^{\frac{1}{4}}}{4\pi^{\frac{3}{2}}} e^{i\sqrt{\lambda - \underline{\beta}\underline{\sigma}}\omega} \otimes \mathcal{X}_\sigma \quad \lambda > \underline{\sigma}\underline{\beta}, \quad (6.19)$$

the map \mathcal{F} is unitary on \mathcal{H} and its inverse is $\mathcal{F}^{-1} : \bigoplus_{\underline{\sigma}} L^2([\underline{\sigma}\underline{\beta}, \infty), \Omega) \rightarrow \mathcal{H}$

$$\mathcal{F}^{-1} \bigoplus_{\underline{\sigma}} \tilde{\psi}^\sigma = \sum_{\underline{\sigma}} \int_{\underline{\sigma}\underline{\beta}}^{\infty} d\lambda \int_{\Omega} d\omega \Phi^\sigma(\lambda, \omega) \tilde{\psi}^\sigma(\lambda, \omega). \quad (6.20)$$

Given $\Psi \in \mathcal{H}_{ac}(H_\alpha)$, the wave operator $W_+^{-1} : \mathcal{H}_{ac}(H_\alpha) \rightarrow \mathcal{H}$ is given by

$$W_+^{-1} = \mathcal{F}^{-1}\mathcal{F}_\alpha. \quad (6.21)$$

Given $\Psi \in \mathcal{H}_{ac}(H_\alpha)$, W_+^{-1} satisfies

$$\lim_{t \rightarrow +\infty} \|e^{-iH_\alpha t}\Psi - e^{-iH_0 t}W_+^{-1}\Psi\| = 0. \quad (6.22)$$

6.3 Asymptotic estimates

Consider the initial state

$$\Psi^0 = \psi^0 \otimes \mathcal{X}_{(-,-)}; \quad \text{with } \psi^0(x) = \psi^0(|x|). \quad (6.23)$$

In our setting $\psi^0(|x|)$ is a spherical wave function traveling out from the origin O .

In the spirit of the result of Mott we want to show that the large-time probability of having both spins flipped is maximal if the spins lie on a straight line passing through the origin. We assume that the initial state is orthogonal to the eigenfunctions of H_α , i.e.,

$$P_{\sigma_{ac}(H_\alpha)}\Psi_0 = \Psi_0. \quad (6.24)$$

Define $\Psi^t := e^{-iH_\alpha t}\Psi^0$, we denote by $\psi_{(+,+)}^t(x)$ the function

$$\psi_{(+,+)}^t(x) := (\Psi^t, \mathcal{X}_{(+,+)}^{\mathbb{C}^2 \otimes \mathbb{C}^2}). \quad (6.25)$$

The asymptotic probability to find both the spin in the state up is

$$\mathcal{P} := \lim_{t \rightarrow +\infty} \|\psi_{(+,+)}^t\|_{L^2}. \quad (6.26)$$

Proposition 1. *Take Ψ^0 like in (6.23). Assume that Ψ^0 satisfies condition (6.24) and that $\text{supp}[\psi^0] \subseteq [0, R]$, with $R < |y_j|$, $j = 1, 2$. Assume moreover that $(|y_1 - y_2|\alpha)^{-1} \ll 1$, $\alpha^2 \gg \beta$ and $|y_2| = |y_1| + \delta$, with $\delta > 0$ and $\delta \ll |y_2|$. Then \mathcal{P} has its maximum in correspondence of the minimum of $|y_1 - y_2|$.*

Proof. Define $\Psi_a^0 := W_+^{-1}\Psi^0$ and $\Psi_a^t := e^{-iH_0 t}\Psi_a^0$.

From formula (6.22) one obtains

$$\lim_{t \rightarrow +\infty} \|\Psi^t - \Psi_a^t\| = \lim_{t \rightarrow +\infty} \sum_{\underline{\sigma}} \|\psi_{\underline{\sigma}}^t(\cdot) - \psi_{a,\underline{\sigma}}^t(\cdot)\|_{L^2} = 0 \quad (6.27)$$

then

$$\lim_{t \rightarrow +\infty} \|\psi_{\underline{\sigma}}^t(\cdot) - \psi_{a,\underline{\sigma}}^t(\cdot)\|_{L^2} = 0 \quad \forall \underline{\sigma} \quad (6.28)$$

Since

$$e^{-iH_0 t}\Psi^0 = \sum_{\underline{\sigma}} U^t \psi_{\underline{\sigma}}^0 \otimes e^{-i\beta \underline{\sigma}} \mathcal{X}_{\underline{\sigma}}, \quad (6.29)$$

with $U^t = e^{-i(-\Delta)t}$, and U^t is unitary in $L^2(\mathbb{R}^3)$

$$\mathcal{P} = \lim_{t \rightarrow +\infty} \|\psi_{(+,+)}^t\|_{L^2} = \lim_{t \rightarrow +\infty} \|\psi_{a,(+,+)}^t\|_{L^2} = \|\psi_{a,(+,+)}^0\|_{L^2} = \|(W_+^{-1}\Psi^0)_{(+,+)}\|_{L^2} \quad (6.30)$$

From the definition of W_+^{-1}

$$\|(W_+^{-1}\Psi^0)_{(+,+)}\|_{L^2} = \int_{\mathbb{R}^3} dx \left| \int_{2\beta}^{+\infty} d\lambda \int_{\Omega} d\omega \phi^{(+,+)}(x; \lambda, \omega) \langle \Phi_{\alpha}^{(+,+)}(\lambda, \omega), \Psi^0 \rangle \right|^2 \quad (6.31)$$

$$= \int_{2\beta}^{+\infty} d\lambda \int_{\Omega} d\omega \left| \langle \Phi_{\alpha}^{(+,+)}(\lambda, \omega), \Psi^0 \rangle \right|^2 \quad (6.32)$$

where

$$\phi^{(+,+)}(x; \lambda, \omega) = \frac{(\lambda - 2\beta)^{\frac{1}{4}}}{4\pi^{\frac{3}{2}}} e^{i\sqrt{\lambda - 2\beta}\omega x}, \quad (6.33)$$

and we used the fact that

$$\int_{\mathbb{R}^3} dx \left| \int_{2\beta}^{+\infty} d\lambda \int_{\Omega} d\omega \phi^{(+,+)}(x; \lambda, \omega) \tilde{f}(\lambda, \omega) \right|^2 = \int_{2\beta}^{+\infty} d\lambda \int_{\Omega} d\omega \left| \tilde{f}(\lambda, \omega) \right|^2 \quad (6.34)$$

From the definition of the generalized eigenfunctions (6.13), we obtain that for $\lambda \geq 2\beta$

$$\langle \Phi_{\alpha}^{(+,+)}(\lambda, \omega), \Psi^0 \rangle = \frac{(\lambda - 2\beta)^{\frac{1}{4}}}{4\pi^{\frac{3}{2}}} \sum_{j, j'} \overline{(\Gamma_{\alpha}(\lambda))}_{j'--, j++}^{-1} e^{-i\sqrt{\lambda-2\beta}\omega y_j} \int_{\mathbb{R}^3} dx \frac{e^{i\sqrt{\lambda+2\beta}|x-y_{j'}|}}{4\pi|x-y_{j'}|} \psi^0(|x|). \quad (6.35)$$

Let us pose

$$F(\lambda; |y_{j'}|) := \int_{\mathbb{R}^3} dx \frac{e^{i\sqrt{\lambda+2\beta}|x-y_{j'}|}}{4\pi|x-y_{j'}|} \psi^0(|x|). \quad (6.36)$$

By a direct calculation one can verify that $(\Gamma_{\alpha}(\lambda))_{1--, 1++}^{-1} = (\Gamma_{\alpha}(\lambda))_{2--, 2++}^{-1}$ and $(\Gamma_{\alpha}(\lambda))_{1--, 2++}^{-1} = (\Gamma_{\alpha}(\lambda))_{2--, 1++}^{-1}$. Let us denote by

$$A(\lambda) := (\Gamma_{\alpha}(\lambda))_{1--, 1++}^{-1} = (\Gamma_{\alpha}(\lambda))_{2--, 2++}^{-1} \quad (6.37)$$

$$B(\lambda) := (\Gamma_{\alpha}(\lambda))_{1--, 2++}^{-1} = (\Gamma_{\alpha}(\lambda))_{2--, 1++}^{-1} \quad (6.38)$$

Under our assumptions on the support of the initial state we obtain

$$F(\lambda; |y_{j'}|) = \frac{e^{i\sqrt{\lambda+2\beta}|y_{j'}|}}{|y_{j'}|} f(\lambda), \quad (6.39)$$

where

$$f(\lambda) := \frac{1}{\sqrt{\lambda+2\beta}} \int_0^R d|x| |x| \sin(\sqrt{\lambda+2\beta}|x|) \psi^0(|x|). \quad (6.40)$$

Then

$$\begin{aligned} |\langle \Phi_{\alpha}^{(+,+)}(\lambda, \omega), \Psi^0 \rangle|^2 &= \frac{|\sqrt{\lambda-2\beta}|}{16\pi^3} |f(\lambda)|^2 \left| A(\lambda) \left(\frac{e^{-i\sqrt{\lambda-2\beta}\omega y_1 + i\sqrt{\lambda+2\beta}|y_1|}}{|y_1|} + \frac{e^{-i\sqrt{\lambda-2\beta}\omega y_2 + i\sqrt{\lambda+2\beta}|y_2|}}{|y_2|} \right) \right. \\ &\quad \left. + B(\lambda) \left(\frac{e^{-i\sqrt{\lambda-2\beta}\omega y_1 + i\sqrt{\lambda+2\beta}|y_2|}}{|y_2|} + \frac{e^{-i\sqrt{\lambda-2\beta}\omega y_2 + i\sqrt{\lambda+2\beta}|y_1|}}{|y_1|} \right) \right|^2 \end{aligned} \quad (6.41)$$

Under the assumption $(|y_1 - y_2|\alpha)^{-1} \ll 1$ one can see that $A(\lambda) = O((|y_1 - y_2|\alpha)^{-2})$ while $B(\lambda) = O((|y_1 - y_2|\alpha)^{-1})$, in particular

$$B(\lambda) = -\frac{e^{-i\sqrt{\lambda}|y_1-y_2|} (4\pi\alpha)^3}{((4\pi\alpha)^2 - \sqrt{\lambda}\sqrt{\lambda+2\beta})((4\pi\alpha)^2 - \sqrt{\lambda}\sqrt{\lambda-2\beta})} \frac{1}{|y_1 - y_2|\alpha} + O((|y_1 - y_2|\alpha)^{-3}). \quad (6.42)$$

By assuming that $|y_2| = |y_1| + \delta$, with $\delta > 0$ and $\delta \ll |y_2|$, and tacking account of the estimate (6.42) one obtains the following estimate for the probability \mathcal{P}

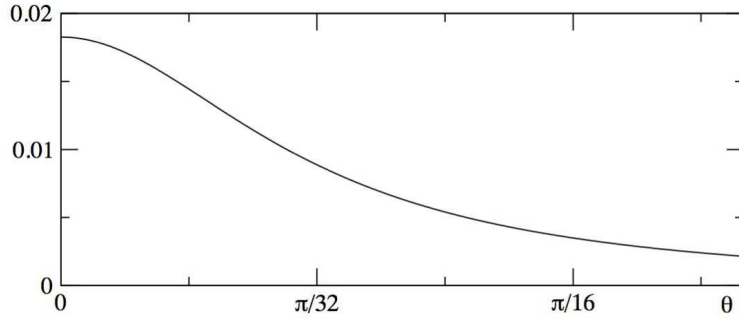
$$\mathcal{P} = \frac{64(4\pi\alpha)^4}{|y_2|^2|y_1 - y_2|^2} \int_{2\beta}^{\infty} \frac{\sqrt{\lambda - 2\beta} |f(\lambda)|^2}{((4\pi\alpha)^2 + \sqrt{\lambda}\sqrt{\lambda + 2\beta})^2 ((4\pi\alpha)^2 + \sqrt{\lambda}\sqrt{\lambda - 2\beta})^2} \times \\ \times \left(1 + \cos(\sqrt{\lambda + 2\beta}\delta) \frac{\sin(\sqrt{\lambda - 2\beta}|y_1 - y_2|)}{\sqrt{\lambda - 2\beta}|y_1 - y_2|} \right) d\lambda + O((|y_1 - y_2|\alpha)^{-3}, (\delta/|y_2|)). \quad (6.43)$$

The statement of the proposition follows from the fact that the function

$$\frac{1}{L^2} \left(1 + \cos(\sqrt{\lambda + 2\beta}\delta) \frac{\sin(\sqrt{\lambda - 2\beta}L)}{\sqrt{\lambda - 2\beta}L} \right) \quad (6.44)$$

is decreasing in L . □

Proposition 1 indicates that if the positions of the spins are such that $|y_2| = |y_1| + \delta$ with $\delta > 0$ and $\delta \ll |y_2|$ then the probability to find both the spins in the state up has a maximum when their distance $y_1 - y_2$ has a minimum. In particular this indicates that if the distances $|y_1|$ and $|y_2|$ are fixed the configuration in which the probability \mathcal{P} has a maximum corresponds to the configuration in which the spin are aligned with the origin.



In figure it is plotted the probability \mathcal{P} when the initial state is of the form

$$\psi^0(|x\rangle) = N \frac{e^{-\frac{|x|^2}{2s^2} + ik_0|x|}}{|x|} \quad N = \frac{1}{\sqrt{2s\pi^{\frac{3}{4}}}}, \quad (6.45)$$

with $s > 0$ and $k_0 > 0$, in a setting in which $|y_1|$ and $|y_2|$ are fixed. On the x -axis of the plot there is the angle θ between y_1 and y_2 , the plot clearly shows that the probability has a maximum when $\theta = 0$

Part III

Resonances

Chapter 7

Resonances

In the last years many important works (see for example [15], [50]) were addressing the study of the spectral properties of non relativistic electrons in a atom, minimally coupled to the quantized electromagnetic field. The main results were: existence and uniqueness of a ground state and that the excited bound states of the unperturbed system become unstable and turn into resonances when the electrons are coupled with the radiation field. Resonances are related to the well known phenomenon of spontaneous emission; in the physics literature this problem is usually analyzed in time dependent perturbation theory, where a periodic potential is chosen to take the role of the electromagnetic interaction. Main results of the theory is the well known Fermi Golden Rule ([70]) expressing the decay rates of the metastable states.

From a mathematical point of view resonances were the object of many investigations ([34], [58], [55]). These studies suggest that the appearance of metastable states comes as a consequence of a perturbation of Hamiltonian with eigenstates embedded in the continuous part of the spectrum. When the perturbation is switched on these eigenvalues can disappear and turn into resonances.

In chapter 5 we characterized a family of selfadjoint Hamiltonians generating the dynamics of a quantum particle interacting, via zero range forces, with an array of localized quantum systems with a finite number of energy levels. With this family of Hamiltonians we can describe and analyze a system made up of a localized quantum bit (a model-atom) in interaction with a non relativistic quantum particle.

The analysis of the appearance of resonances and their time decay will proceed as follows. First we define an “unperturbed” Hamiltonian H_α belonging to the family we introduced in chapter 5. We chose parameters in H_α in such a way that the spectrum of H_α has one eigenvalue embedded in the continuous spectrum. Then we define Hamiltonian H_ϵ , always in the same family, that are small perturbations (in resolvent sense) of H_α . We will show that the ground state move slightly in energy and the embedded eigenvalue moves into a res-

onance. Finally we estimate the decay times of such resonances.

It is shown that all the various characterizations of resonances discussed recently [34], [58], [55] apply in our model. The extension of our results to any multilevel localized system is straightforward. The generalization to the case of a large number of non relativistic particles interacting with the localized q-bit seems straightforward and is in progress. The model discussed here appears as a simplified non-relativistic version of the system analyzed in [15], [50]. In spite of their simplicity the Hamiltonians we define in the following show interesting spectral features considered to be typical of more complex and realistic systems.

7.1 Notation

In this section we review notation and results of chapter 5 when the quantum system consists of one particle interacting with one spin.

A localized two levels system is well depicted by a spin 1/2 placed in a fixed position of space, i.e. a unitary vector in \mathbb{C}^2 . Without losing ingenerality we assume that the spin is placed in $y = 0$. The state of the spin is represented by a linear superposition $a\chi_+ + b\chi_-$, with $a, b \in \mathbb{C}$ and $|a|^2 + |b|^2 = 1$.

The natural Hilbert space for a system made up of one particle in dimension d and one spin 1/2 is

$$\mathcal{H} := L^2(\mathbb{R}^d) \otimes \mathbb{C}^2 \quad d = 1, 2, 3. \quad (7.1)$$

We denote by a capital Greek letter the generic vector in \mathcal{H} . $\Psi \in \mathcal{H}$ can be written in the following form

$$\Psi = \sum_{\sigma} \psi_{\sigma} \otimes \chi_{\sigma}, \quad (7.2)$$

where the sum runs over $\sigma = \pm$.

Hamiltonians H_{α} and H_{ϵ} will be defined as self-adjoint extensions of an assigned symmetric operator, in the way we presented in chapter 5 (see Theorem 5.2.1, Theorem 5.2.2 and Theorem 5.2.3), relative to suitable choices of matrices A and B .

7.2 Unperturbed Hamiltonian

Definition 1. Let $-\infty < \alpha \leq \infty$, then

$$D(H_{\alpha}) := \left\{ \Psi \in \mathcal{H} \mid \Psi = \Psi^z + \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z; \Psi^z = \sum_{\sigma} \psi_{\sigma}^z \otimes \chi_{\sigma} \in D(H_0); z \in \rho(H_{\alpha}); \right. \\ \left. q_{\sigma} = -\alpha f_{\sigma}, d = 1; \alpha q_{\sigma} = f_{\sigma}, d = 2; \alpha q_{\sigma} = f_{\sigma}, d = 3 \right\} \quad (7.3)$$

$$H_\alpha \Psi := H_0 \Psi^z + z \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z \quad \Psi \in D(H_\alpha). \quad (7.4)$$

Self-adjointness of H_α comes directly from Theorem 5.2.1, Theorem 5.2.2 and Theorem 5.2.3 by taking $A = \mathbb{I}_2$ and $B = -\alpha \mathbb{I}_2$ for $d = 1$, $A = \alpha \mathbb{I}_2$ and $B = \mathbb{I}_2$ for $d = 2, 3$. In this way the Hamiltonian H_α defines a dynamics such that the particle “feels” the qubit as a δ -like potential of strength α centered in $x = 0$. The explicit formula for resolvent of H_α , as it was given in chapter 5, reads

$$R_\alpha(z) = R(z) + \sum_{\sigma, \sigma'} ((\Gamma_0(z))^{-1})_{\sigma, \sigma'} \langle \Phi_{\sigma'}^z, \cdot \rangle \Phi_{\sigma}^z \quad z \in \mathbb{C} \setminus \mathbb{R}, \quad (7.5)$$

where $R(z) = (H_0 - z)^{-1}$ (H_0 is defined in (5.9)) and

$$\Gamma_\alpha(z) = \begin{pmatrix} -\frac{i}{2\sqrt{z-\beta}} - \frac{1}{\alpha} & 0 \\ 0 & -\frac{i}{2\sqrt{z+\beta}} - \frac{1}{\alpha} \end{pmatrix} \quad d = 1 \quad (7.6)$$

$$\Gamma_\alpha(z) = \begin{pmatrix} \frac{\ln(\sqrt{z-\beta}/2) + \gamma - i\pi/2}{2\pi} + \alpha & 0 \\ 0 & \frac{\ln(\sqrt{z+\beta}/2) + \gamma - i\pi/2}{2\pi} + \alpha \end{pmatrix} \quad d = 2 \quad (7.7)$$

$$\Gamma_\alpha(z) = \begin{pmatrix} \frac{\sqrt{z-\beta}}{4\pi i} + \alpha & 0 \\ 0 & \frac{\sqrt{z+\beta}}{4\pi i} + \alpha \end{pmatrix} \quad d = 3. \quad (7.8)$$

Let us characterize the spectrum of H_α

Theorem 7.2.1 (Spectrum of H_α). *For $d = 1, 2, 3$ the essential spectrum¹ is given by*

$$\sigma_{\text{ess}}(H_\alpha) = [-\beta, +\infty). \quad (7.9)$$

For $d = 1, 2, 3$ the point spectrum is given by the real roots of equation $\det \Gamma_\alpha(z) = 0$.

$d = 1$. If $0 \leq \alpha < \infty$ the point spectrum is empty. If $-\infty < \alpha < 0$ the point spectrum consists of two simple eigenvalues given by

$$E_{\alpha,-} = -\beta - \frac{\alpha^2}{4}; \quad E_{\alpha,+} = \beta - \frac{\alpha^2}{4}. \quad (7.10)$$

¹For a definition of essential spectrum see [75], pg 236.

For all $-\infty < \alpha < 0$ the lowest eigenvalue, $E_{\alpha,-}$, is below the threshold of the essential spectrum. For $\alpha < -2\sqrt{2\beta}$ also the second eigenvalue, $E_{\alpha,+}$, is below the threshold of the essential spectrum, in such a case the point spectrum is only discrete and the essential spectrum is only absolutely continuous. If $-2\sqrt{2\beta} \leq \alpha < 0$ the upper eigenvalue is embedded in the continuous spectrum, $-\beta \leq E_{\alpha,+} < \beta$.

$d = 2$. For all $-\infty < \alpha < \infty$ the point spectrum consists of two simple eigenvalues given by

$$E_{\alpha,-} = -\beta - 4e^{-2(2\pi\alpha+\gamma)}; \quad E_{\alpha,+} = \beta - 4e^{-2(2\pi\alpha+\gamma)}. \quad (7.11)$$

The lowest eigenvalue, $E_{\alpha,-}$, is always below the threshold of the essential spectrum. For $-\infty < \alpha < -(\ln(\sqrt{\beta/2}) + \gamma)/(2\pi)$ also the second eigenvalue, $E_{\alpha,+}$, is below the threshold of the essential spectrum, in such a case the point spectrum is only discrete and the essential spectrum is only absolutely continuous. If $-(\ln(\sqrt{\beta/2}) + \gamma)/(2\pi) \leq \alpha < \infty$ the second eigenvalue is embedded in the continuous spectrum, $-\beta \leq E_{\alpha,+} < \beta$.

$d = 3$. If $0 \leq \alpha < \infty$ the point spectrum is empty. If $-\infty < \alpha < 0$ the point spectrum consists of two simple eigenvalues given by

$$E_{\alpha,-} = -\beta - (4\pi\alpha)^2; \quad E_{\alpha,+} = \beta - (4\pi\alpha)^2. \quad (7.12)$$

The lowest eigenvalue, $E_{\alpha,-}$, is always below the threshold of essential spectrum. For $-\infty < \alpha < -\sqrt{2\beta}/(4\pi)$ also the second eigenvalue, $E_{\alpha,+}$, is below the threshold of essential spectrum, in such a case the point spectrum is only discrete and the essential spectrum is only absolutely continuous. If $-\sqrt{2\beta}/(4\pi) \leq \alpha < 0$ the second eigenvalue is embedded in the continuous spectrum, $-\beta \leq E_{\alpha,+} < \beta$.

Proof.

The spectrum of H_α is easily obtained from (7.5) and from the spectral structure of the "free" Schrödinger operator H_0 . The Weyl's theorem ([75], p.112) imply that the essential spectrum of H_α and H_ϵ coincides. The point spectrum of H_0 is empty, and from the resolvent we have that the point spectrum is given only by the zeros of the determinant of $\Gamma_\alpha(z)$. □

Let us assume that, in any dimension, parameters are chosen so that there are two eigenvalues and that the upper one is embedded in the continuous part of the spectrum, like in the following figure

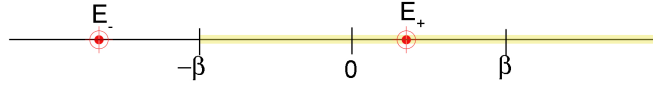


Figure 7.1: The bound state $E_{\alpha,-}$ is below the threshold of the continuous spectrum where the eigenvalue $E_{\alpha,+}$ is embedded

7.3 Turning to resonances, perturbation of the diagonal interaction

In the same way as we did for H_α we define H_ϵ

Definition 2 (H_ϵ). Let $-\infty < \alpha \leq \infty$ and $0 < \epsilon \ll \alpha$, then

$$D(H_\epsilon) := \left\{ \Psi \in \mathcal{H} \mid \Psi = \Psi^z + \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z; \Psi^z = \sum_{\sigma} \psi_{\sigma}^z \otimes \chi_{\sigma} \in D(H_0); z \in \rho(H_\epsilon); \right. \\ \left. \begin{aligned} q_{\pm} &= -\alpha f_{\pm} - \epsilon f_{\mp} & d = 1; \\ \alpha q_{\pm} + \epsilon q_{\mp} &= f_{\pm} & d = 2; \\ \alpha q_{\pm} + \epsilon q_{\mp} &= f_{\pm} & d = 3 \end{aligned} \right\} \quad (7.13)$$

$$H_\epsilon \Psi := H_0 \Psi^z + z \sum_{\sigma} q_{\sigma} \Phi_{\sigma}^z \quad \Psi \in D(H_\epsilon). \quad (7.14)$$

Let us consider a perturbation of H_0, H_ϵ such that the operator H_ϵ is self-adjoint and its resolvent, $R_\epsilon(z) := (H_\epsilon - z)^{-1}$, is given by

$$R_\epsilon(z) = R(z) + \sum_{\sigma, \sigma'} ((\Gamma_\epsilon(z))^{-1})_{\sigma, \sigma'} \langle \Phi_{\sigma'}^z, \cdot \rangle \Phi_{\sigma}^z \quad z \in \rho(H_\epsilon), \quad (7.15)$$

where

$$\Gamma_\epsilon(z) := \begin{pmatrix} \frac{1}{2i\sqrt{z-\beta}} - \frac{1}{\alpha} & \epsilon \\ \epsilon & \frac{1}{2i\sqrt{z+\beta}} - \frac{1}{\alpha} \end{pmatrix} \quad d = 1 \quad (7.16)$$

$$\Gamma_\epsilon(z) = \begin{pmatrix} \frac{1}{2\pi} \ln \frac{\sqrt{\eta(z-\beta)}}{i} & i\epsilon \\ -i\epsilon & \frac{1}{2\pi} \ln \frac{\sqrt{\eta(z+\beta)}}{i} \end{pmatrix} \quad d = 2$$

$$\Gamma_\epsilon(z) = \begin{pmatrix} \frac{\sqrt{z-\beta}}{4\pi i} - \alpha & i\epsilon \\ -i\epsilon & \frac{\sqrt{z+\beta}}{4\pi i} - \alpha \end{pmatrix} \quad d = 3$$

with C real constant.

Comparing (7.5) and (7.15) it is clear that H_ϵ has a resolvent that is a small perturbation of the resolvent H_α . In the next section we study the modification of the spectral structure due to the perturbation.

Resonances

In the following the spectral properties of H_ϵ near $E_{\alpha,+}$ are analyzed when ϵ is "small enough" in a sense that will depend on the dimension. In $d = 3$ we will mean that $\epsilon^2/|\alpha|^2 \ll 1$.

Eigenvalues of H_ϵ are real solutions of equation $\det \Gamma_\epsilon(\lambda) = 0$.

It is very easy to check that a real solutions λ of the equation is a continuous function of ϵ moving slightly from its position $E_{\alpha,-}$ from $\epsilon = 0$.

Up to the second order in ϵ^2

$$\lambda = E_{\alpha,-} - \frac{64\pi^3\alpha^2}{\beta} : \epsilon^2$$

We are interested in what happens around $E_{\alpha,+}$. To this aim we consider only the values of λ in the interval $-\beta < \lambda < \beta$. We will give details only for the case $d = 3$.

In this case we have to solve

$$(i\sqrt{\lambda - \beta} + 4\pi\alpha)(i\sqrt{\lambda + \beta} + 4\pi\alpha) + (4\pi\epsilon)^2 = 0. \quad (7.17)$$

taking into account the signum of the imaginary part of the square root we can rewrite the (7.17) as

$$-i\sqrt{\beta^2 - \lambda^2} - 4\pi\alpha\sqrt{\beta - \lambda} + 4\pi\alpha + i\sqrt{\beta + \lambda} + (4\pi)^2(\alpha^2\epsilon^2) = 0$$

which can be easily showed that have no zeros between $-\beta$ and β with $\epsilon \neq 0$

Let us look for complex solutions of the eigenvalue equation

$$\left(\frac{\sqrt{\beta - \lambda}}{4\pi} - \alpha\right)\left(\frac{\sqrt{\beta + \lambda}}{4\pi i} - \alpha\right) = \epsilon^2 \quad (7.18)$$

With the following position

$$\xi = \left(\frac{\sqrt{\beta - \lambda}}{4\pi} - \alpha\right) \quad \eta = -\left(\frac{\sqrt{\beta + \lambda}}{4\pi i} - \alpha\right)$$

the equation reads

$$\xi = -\frac{\epsilon^2}{\eta}$$

We define the following recurrence procedure

$$\xi = 0 \Rightarrow \begin{cases} \lambda_0 = \beta - (4\pi\alpha)^2 \\ \eta_0 = i\frac{\sqrt{2\beta - (4\pi\alpha)^2}}{4\pi} + \alpha \end{cases} \quad \begin{cases} \xi_k = -\frac{\epsilon^2}{\eta_k} \\ \eta_k = \alpha + i\frac{\sqrt{2\beta - [4\pi(\xi_{k-1}\alpha)]^2}}{4\pi} \end{cases} \quad (7.19)$$

From the definition we have that $|\eta_k| > \alpha$ and $|\xi_k| < \frac{\epsilon^2}{\alpha}$ and being

$$\xi_{k+1} - \xi_k = \frac{\epsilon^2}{\eta_k \eta_{k+1}} (\eta_{k+1} - \eta_k)$$

we also have

$$|\xi_{k+1} - \xi_k| \leq \frac{\epsilon^2}{\alpha^2} |\eta_{k+1} - \eta_k| \quad (7.20)$$

Now we use the following estimate

$$\sqrt{2\beta - p^2} - \sqrt{2\beta - q^2} = \int_p^q \frac{s}{\sqrt{2\beta - s^2}} ds \leq |p - q| \sup(p, q) \sup\left(\frac{1}{\sqrt{2\beta - s^2}}\right)$$

to obtain

$$\begin{aligned} |\eta_{k+1} - \eta_k| &= \left| \frac{\sqrt{2\beta - [4\pi(\xi_k\alpha)]^2}}{4\pi} - \frac{\sqrt{2\beta - [4\pi(\xi_{k-1}\alpha)]^2}}{4\pi} \right| \\ &\leq |\xi_k - \xi_{k-1}| \frac{\epsilon^2}{\alpha} C \end{aligned} \quad (7.21)$$

From (5) and (6)

$$|\xi_{k+1} - \xi_k| \leq \frac{\epsilon^2}{\alpha^2} |\eta_{k+1} - \eta_k| \leq |\xi_k - \xi_{k-1}| \frac{\epsilon^4}{\alpha^3} C$$

Summing the series

$$|\xi_\infty - \xi_0| \leq \frac{|\xi_1 - \xi_0|}{1 - \frac{C\epsilon^4}{\alpha^3}}$$

with

$$\xi_1 - \xi_0 = \frac{4\pi i\alpha}{\sqrt{2\beta - (4\pi\alpha)^2} \left(\alpha + \frac{i}{4\pi} \sqrt{2\beta - (4\pi\alpha)^2} \right)^3} \epsilon^4 + O(\epsilon^6)$$

At the first order

$$\xi_0 = -\frac{\epsilon^2}{\eta_0} = -\frac{\epsilon^2 \left(\alpha - \frac{i\sqrt{2\beta - (4\pi\alpha)^2}}{4\pi} \right)}{2\beta}$$

so that at the order ϵ^2 the location of the zero is

$$\begin{aligned}\lambda_{res} &= \beta - [4\pi(\xi + \alpha)]^2 \\ &= \beta - (4\pi\alpha)^2 \left[1 - \frac{(4\pi\alpha\epsilon)^2}{\beta} \right] - i\frac{\alpha}{\beta}(4\pi)^3\sqrt{2\beta - (4\pi\alpha)^2}\epsilon^2 \\ &= x_0 - i\gamma\end{aligned}$$

with a negative imaginary part.

Notice that the result comes from an expansion on the real axis of $\sqrt{\beta - z}$ around $E_{0,+}$. A negative imaginary part of the result means that the solution λ is in the second Riemann sheet, just below the real axis ($\arg(\lambda) \simeq 4\pi$). The analysis of resonances can be done also using numerical methods. In this way we have obtained the following plots showing the value of the imaginary part of the resonances as function of ϵ for $d = 1, 2, 3$

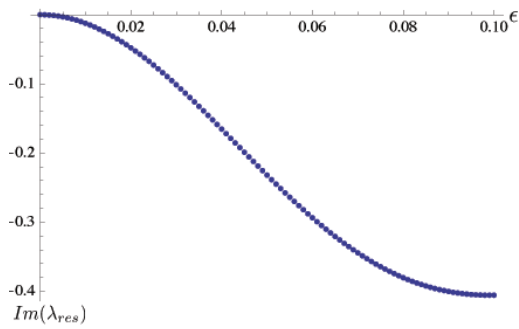


Figure 7.2: Imaginary part of λ_{res} as function of ϵ in \mathbb{R}^3

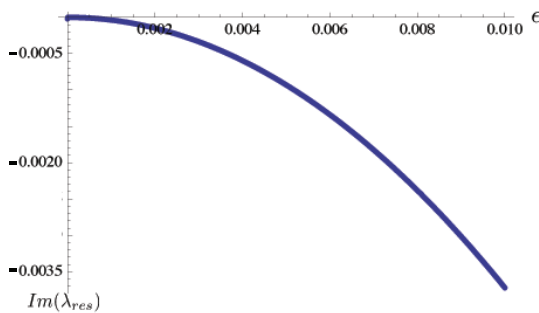


Figure 7.3: Imaginary part of λ_{res} as function of ϵ in \mathbb{R}^2

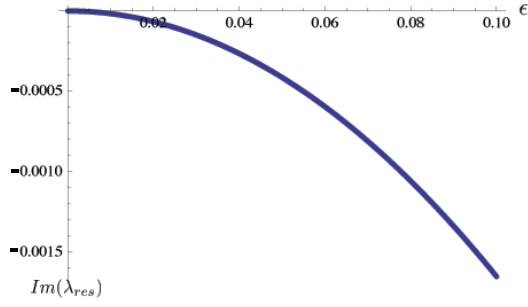


Figure 7.4: Imaginary part of λ_{res} as function of ϵ in \mathbb{R}

7.4 Exponential Decay

We started with an Hamiltonian with two true eigenvalues, one of which embedded in the continuous part of the spectrum. The time evolution relative to the Hamiltonian H_α of the relative eigenstate would amount to a phase factor. When we switch on the perturbation we proved, in dimension $d = 3$, that this eigenvalue “becomes complex”. The name given to “complex eigenvalues” close to real axis, in the second Riemann sheet, is resonances. The presence of resonances strongly modifies the local structure of the spectral density giving important effects in a scattering event around that energy.

We will analyze this problem in a specific case. Again we limit the details to the case $d = 3$.

From the explicit form of the resolvent we obtain the following expression for the generalized eigenfunctions of H_ϵ (the bounded solutions of $(H_\epsilon - \lambda)\Phi^\lambda = 0$):

$$\Phi_{(1)}^\lambda(\omega) = \frac{\sqrt{\lambda - \beta}}{4\pi^{3/2}} \left[e^{i\omega\sqrt{\lambda - \beta}x} \otimes \chi_+ + \frac{\frac{\sqrt{\lambda + \beta}}{4\pi i} - \alpha}{\left(\frac{\sqrt{\lambda - \beta}}{4\pi i} - \alpha\right)\left(\frac{\sqrt{\lambda + \beta}}{4\pi i} - \alpha\right) - \epsilon^2} \frac{e^{i\sqrt{\lambda - \beta}|x|}}{4\pi|x|} \otimes \chi_{++} + \frac{i\epsilon}{\left(\frac{\sqrt{\lambda - \beta}}{4\pi i} - \alpha\right)\left(\frac{\sqrt{\lambda + \beta}}{4\pi i} - \alpha\right) - \epsilon^2} \frac{e^{i\sqrt{\lambda + \beta}|x|}}{4\pi|x|} \otimes \chi_- \right] \quad \lambda > \beta, \omega \in S^2$$

$$\Phi_{(2)}^\lambda(\omega) = \frac{\sqrt{\lambda + \beta}}{4\pi^{3/2}} \left[e^{i\omega\sqrt{\lambda + \beta}x} \otimes \chi_- + \frac{\frac{\sqrt{\lambda - \beta}}{4\pi i} - \alpha}{\left(\frac{\sqrt{\lambda - \beta}}{4\pi i} - \alpha\right)\left(\frac{\sqrt{\lambda + \beta}}{4\pi i} - \alpha\right) - \epsilon^2} \frac{e^{i\sqrt{\lambda + \beta}|x|}}{4\pi|x|} \otimes \chi_{-+} + \frac{i\epsilon}{\left(\frac{\sqrt{\lambda - \beta}}{4\pi i} - \alpha\right)\left(\frac{\sqrt{\lambda + \beta}}{4\pi i} - \alpha\right) - \epsilon^2} \frac{e^{i\sqrt{\lambda - \beta}|x|}}{4\pi|x|} \otimes \chi_+ \right] \quad \lambda > -\beta, \omega \in S^2$$

We have all the ingredients to compute the probability that the system evolve remaining in a small range of energy of amplitude Δ around $E_{\alpha,+}$

$$\begin{aligned}
P_{++}^{\Delta}(t) &= \int_{\Delta} \frac{\epsilon^2 e^{-i\lambda t}}{\left| \left(\frac{\sqrt{\beta-\lambda}}{4\pi} - \alpha \right) \left(\frac{\sqrt{\beta+\lambda}}{4\pi i} - \alpha \right) - \epsilon^2 \right|^2} \frac{e^{-2\sqrt{\beta-\lambda}|x|}}{16\pi^2|x|^2} d\lambda \\
&= \frac{\epsilon^2}{(4\pi|x|)^2} \int_{\Delta} \frac{e^{-i\lambda t} e^{-2\sqrt{\beta-\lambda}|x|}}{\left(\left(\frac{\sqrt{\beta-\lambda}}{4\pi} - \alpha \right) \left(\frac{\sqrt{\beta+\lambda}}{4\pi i} - \alpha \right) - \epsilon^2 \right) \left(\left(\frac{\sqrt{\beta-\lambda}}{4\pi} - \alpha \right) \left(\frac{-\sqrt{\beta+\lambda}}{4\pi i} - \alpha \right) - \epsilon^2 \right)} d\lambda \\
&= \frac{\epsilon^2}{(4\pi|x|)^2} \int_{\Delta} \frac{h(\lambda)}{f(\lambda)g(\lambda)} d\lambda
\end{aligned} \tag{7.22}$$

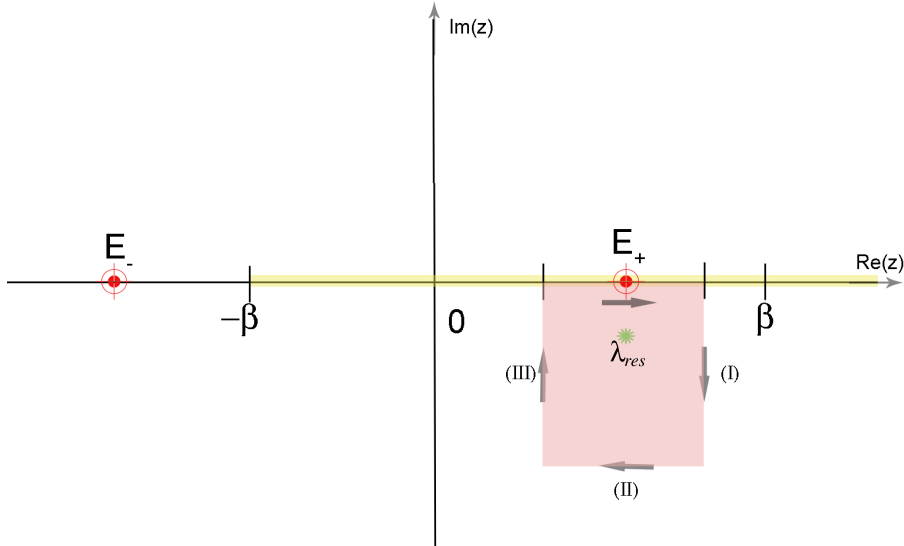
where

$$f(\lambda) = \left(\frac{\sqrt{\beta-\lambda}}{4\pi} - \alpha \right) \left(\frac{\sqrt{\beta+\lambda}}{4\pi i} - \alpha \right) - \epsilon^2 \tag{7.23}$$

$$g(\lambda) = \left(\frac{\sqrt{\beta-\lambda}}{4\pi} - \alpha \right) \left(-\frac{\sqrt{\beta+\lambda}}{4\pi i} - \alpha \right) - \epsilon^2 \tag{7.24}$$

$$h(\lambda) = e^{-i\lambda t} e^{-2\sqrt{\beta-\lambda}|x|} \tag{7.25}$$

and Δ is a small energy interval around $E_{\alpha,+}$. We evaluate the integral in the last term of (7.22) extending the integrand in the bottom complex plane following the trip in figure.



It is very easy to see that the integral along the path in the lower complex plane is of order $\epsilon^2 \Delta$ so that the only non negligible contribution comes from the pole

inside the circuit:

$$2\pi i \operatorname{Res}_{z=(x_0-i\gamma)} \left[\frac{h(z)}{f(z)g(z)^*} \right] = 2\pi i \frac{h(\lambda_{res})}{\left. \frac{df}{d\lambda} \right|_{\lambda=\lambda_{res}}} g(\lambda_{res}) = A e^{-i x_0 t} e^{-\gamma t}$$

$$A = \frac{(2\pi i) e^{-2\sqrt{\beta-x_0+i\gamma}|x|}}{\left[\frac{\gamma+ix_0}{(4\pi)^2 \sqrt{\beta^2-x_0^2-\gamma^2}} + \frac{\alpha}{8\pi} \left(\frac{i}{\sqrt{\beta+x_0-i\gamma}} + \frac{1}{\sqrt{\beta-x_0+i\gamma}} \right) \right] \left[\left(\frac{\sqrt{\beta-x_0-i\gamma}}{4\pi} - \alpha \right) \left(\frac{\sqrt{\beta+x_0+i\gamma}}{4\pi i} - \alpha \right) - \epsilon^2 \right]}$$

Notice the typical decaying behavior with a decay time of order $1/\epsilon^2$ given by the inverse of the imaginary part of the position of the pole.

Summarizing we proved that of the two state of the unperturbed “atom” only the ground state survives whereas the one embedded in the continuous part of the spectrum becomes a metastable state with a lifetime explicitly computable from the parameters of the model.

Chapter 8

Conclusions

In this thesis we have presented models of quantum dynamics of systems conventionally divided into a *microscopic* quantum subsystem and a *large* quantum system called the environment. Main features we wanted to focus on was the diffusion of quantum correlations into the environment and the reduced dynamics of the subsystem. Our main purpose was the analysis of the specific process of information transfer, produced by the interaction between subsystems, which leads to an evolution from an initial pure state to a final statistical mixture.

Our choice has been to investigate the dynamics for the whole system given by the Schrödinger equation without any statistical assumption on the effects of the interaction of the environment with the microscopic subsystem. This choice forced us to analyze oversimplified models with very elementary dynamical behavior. In particular we used *solvable* interaction, which means Hamiltonians whose spectral properties are known in detail.

First we have analyzed one heavy particle interacting with an environment made up of light particles. We proved a rigorous version of the so called Joos and Zeh formula describing the dynamical transition induced by a single scattering event between the heavy and one of the light particles. We were able to compute the specific error one makes in using this formula instead of the complete dynamics. We have used our results in order to study the decoherence phenomenon induced by the interaction: we considered an heavy particle, with an initial state in a coherent superposition of two wave packets centered symmetrically around the origin in position $-R_0$ and R_0 with momentum $-P_0$ and P_0 , and a light particle at rest at the origin. Assuming a factorized initial state for the whole system we obtained an estimate for the loss of visibility of the interference pattern, after tracing out the light particle degrees of freedom.

Those results were published in [43] and [27].

The decoherence effect is supposed to grow exponentially with the number of particles of the environment interacting with the subsystem under study.

Being systems of many particles well out of reach of any analytical investigation, our idea, borrowed from the techniques of quantum information theory, was to consider the simplest quantum environments able to pick up informations from the subsystem under observation and affecting in the most negligible way the state of the subsystem. To this aim we developed a new scheme of interaction between a particle and an array of spins, via point interactions (see [28] where our results were published)

With this technical tool we worked out a model for a tracking chamber. It is well known that, when revealed by detectors, quantum particles exhibit classical properties. This phenomenon was first investigated by N.F.Mott in 1929: he studied a model able to explain the formation of straight lines in a α -decay experiment. Mott deduced that the tracks were the consequence of the interaction between the α -particle and the environment. Using the results of our work we gave a non perturbative proof of the Mott's conjecture (see [29]).

In the last part of the thesis we presented a simple model for the formation of metastable states.

Metastable states are connected with the phenomenon of spontaneous emission. It is well known that electrons in the excited level of an atom make transitions to the ground state emitting radiation. The connection of this mechanism with the interaction with the quantized radiation field is definitively subtle. The problem is usually addressed via a semiclassical model: a quantum system with fixed energy levels is perturbed by a time dependent potential. Using perturbation theory is possible to evaluate the decay rates of the metastable states (Fermi Golden Rule).

During last years serious attempts to analyze the complete quantum system successfully detailed the entire mechanism. Due to overwhelming technical difficulties, it is very complicate to read the results and almost impossible to use them in applications.

The mechanism was also analyzed in many mathematical papers: the mechanism suggested is that states embedded in the continuous spectrum of the whole system because of the perturbation turn these into resonances, characterized by a slow exponential decay.

Using point interaction Hamiltonians we were able to define a class of systems made up of a model atom interacting with a particle. In the family of selfadjoint operators we can pick up "unperturbed" Hamiltonians with two energy levels: a ground state under the threshold of the continuous spectrum where the other eigenvalue is embedded. In the same family we can define perturbed Hamiltonians and study their spectral properties.

Within this model we can analyze the formation of resonances and evaluate the transition rate in an explicit way using a non perturbative approach.

The preliminary results contained in chapter seven can be easily generalized in two different directions:

- extensions of our results to a multilevel localized system
- generalization to the case of a large number of non relativistic particles interacting with the localized q-bit

Non trivial models of metastable states are required in many fields of fundamental and applied Quantum Mechanics. In particular we intend to use our results to investigate a phenomenon which has been attracting much attention in quantum physics in the last years: the quantum Zeno effect, the tendency to the freezing of the dynamics induced in a quantum system by frequent measurements.

Appendix A

Proof of Theorem 4.0.1

Following the same line as in [38] and [5] we prove theorem 4.0.1 in three steps each one consisting in the proof of a lemma.

Lemma 1. *If condition A is satisfied then there exists a constant $C_1 > 0$ such that, for any $t \in \mathbb{R}^+$ one has*

$$\|\Psi^\varepsilon(t) - \Psi_1^\varepsilon(t)\| \leq C_1 \varepsilon \quad (\text{A.1})$$

where we defined

$$\begin{aligned} \Psi_1^\varepsilon(t; R, r) \equiv & \int_{\mathbb{R}^6} dx' dy' e^{-i\frac{t}{1+\varepsilon}H_0} \left(\frac{R + \varepsilon r}{1 + \varepsilon} - x' \right) \varphi(x') \times \\ & \times e^{-i\frac{t(1+\varepsilon)}{\varepsilon}H_\alpha} (r - R, y') \chi(y' + x') \end{aligned} \quad (\text{A.2})$$

Proof. Notice that $\Psi^\varepsilon(t)$ is the result of the evolution generated by the Hamiltonian H^ε 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

$$\|\Psi^\varepsilon(t) - \Psi_1^\varepsilon(t)\|^2 = \|\Psi^\varepsilon(0) - \Psi_1^\varepsilon(0)\|^2 = \quad (\text{A.3})$$

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

We get then the following estimate

$$\|\Psi^\varepsilon(0) - \Psi_1^\varepsilon(0)\|^2 \leq \varepsilon^2 \int_{\mathbb{R}^6} dx dy |y|^2 |\nabla_x (\varphi(x) \chi(x + y))|^2 \quad (\text{A.5})$$

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

$$C_1^2 \equiv \int_{\mathbb{R}^6} dx dy |y|^2 |\nabla_x (\varphi(x) \chi(x + y))|^2 \quad (\text{A.6})$$

□

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

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

where

$$\begin{aligned} \Psi_2^\varepsilon(t; R, r) &\equiv \int_{\mathbb{R}^3} dx' e^{-i\frac{t}{1+\varepsilon}H_0} \left(\frac{R + \varepsilon r}{1 + \varepsilon} - x'\right) \varphi(x') \times \\ &\times \int_{\mathbb{R}^3} dy' e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0} (r - R - y') [\Omega_+^{-1}\chi(\cdot + x')] (y') \end{aligned} \quad (\text{A.8})$$

Proof. Following the notation of [5] we define $\chi_x(y) \equiv \chi(x + y)$. By direct computation we have

$$\begin{aligned} \|\Psi_2^\varepsilon(t) - \Psi_1^\varepsilon(t)\|^2 &= \int_{\mathbb{R}^6} dx dy \left| \int_{\mathbb{R}^6} dx' dy' e^{-i\frac{t}{1+\varepsilon}H_0} (x - x') \varphi(x') \times \right. \\ &\times \left. \left[e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0} (y - y') [\Omega_+^{-1}\chi_{x'}] (y') - e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0} (y, y') \chi_{x'}(y') \right] \right|^2 \end{aligned} \quad (\text{A.9})$$

Define the unitary operator $\Omega_\tau^+ = e^{i\tau H_\alpha} e^{-i\tau H_0}$ and its inverse $(\Omega_\tau^+)^{-1} = e^{i\tau H_0} e^{-i\tau H_\alpha}$. Using the unitarity of the free propagator e^{-itH_0} we obtain

$$\|\Psi_2^\varepsilon(t) - \Psi_1^\varepsilon(t)\|^2 = \int_{\mathbb{R}^3} dx |\varphi(x)|^2 \int_{\mathbb{R}^3} dy \left| [\Omega_+^{-1}\chi_x] (y) - \left[\left(\Omega_{\frac{1+\varepsilon}{\varepsilon}t}^+\right)^{-1} \chi_x \right] (y) \right|^2 \quad (\text{A.10})$$

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

$$\|(\Omega_+^{-1} - (\Omega_\tau^+)^{-1}) \chi\|_{L^2(\mathbb{R}^3)} = \|(\Omega_+ - \Omega_\tau^+) \Omega_+^{-1} \chi\|_{L^2(\mathbb{R}^3)} \quad (\text{A.11})$$

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

$$\|(\Omega_+ - \Omega_\tau^+) \eta\|_{L^2(\mathbb{R}^3)} \leq \frac{C'}{\tau^{\frac{3}{4}}} \quad \text{for } \tau \rightarrow \infty \quad (\text{A.12})$$

In fact from (3.30) we have

$$[\Omega_+ \eta](x) = [\mathcal{F}_+^{-1} \mathcal{F} \eta](x) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^6} dk dy \Phi_+(x, k) e^{-iky} \eta(y) \quad (\text{A.13})$$

whereas from its definition

$$[\Omega_\tau^+ \eta](y) = \int_{\mathbb{R}^6} dz dy' e^{i\tau H_\alpha}(y, z) e^{-i\tau H_0}(z - y') \eta(y') \quad (\text{A.14})$$

By explicit computation we have

$$(\Omega_+ - \Omega_\tau^+) \eta = W_0 \eta + W_\alpha \eta \quad (\text{A.15})$$

with

$$[W_0 \eta](|x|) = \frac{2i}{(2\pi)^2} \frac{1}{|x|} \int_0^\infty \frac{1 - e^{-i\frac{|x|^2 - |y|^2}{4\tau}}}{|x|^2 - |y|^2} g(|y|) d|y| \quad (\text{A.16})$$

and

$$[W_\alpha \eta](|x|) = \frac{8\pi i \alpha}{(2\pi)^2} \frac{1}{|x|} \int_0^\infty d|y| \frac{g(|y|)}{|y|} \int_0^\infty ds e^{-is|x|} \sin s|y| \times \left(\frac{1}{4\pi\alpha + is} - e^{-i\frac{|x|^2 - |y|^2}{4\tau}} \sqrt{-i\pi\tau} e^{z^2} \operatorname{erfc}(z) \right) \quad (\text{A.17})$$

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 (A.16) we have

$$\|W_0 \eta\|_{L^2(\mathbb{R}^3)}^2 \leq \frac{16}{(2\pi)^3} \int_0^\infty |g(|y|)|^2 K_\tau(|y|) d|y| \quad (\text{A.18})$$

where

$$K_\tau(|y|) = \frac{1}{16\tau^{\frac{3}{2}}} \int_0^\infty \frac{1 - \cos\left(\xi - \frac{|y|^2}{4\tau}\right)}{\left(\xi - \frac{|y|^2}{4\tau}\right)^2} \frac{1}{\sqrt{\xi}} d\xi \leq \frac{1}{16\tau^{\frac{3}{2}}} \left[2 + \sqrt{\frac{|y|^2}{4\tau} + 1} \right] \quad (\text{A.19})$$

We obtain then

$$\|W_0 \eta\|_{L^2(\mathbb{R}^3)}^2 \leq D_0 \left[\frac{1}{\tau^{\frac{3}{2}}} \int_0^\infty |g(|y|)|^2 d|y| + \frac{1}{\tau^2} \int_0^\infty |g(|y|)|^2 |y| d|y| \right] \quad (\text{A.20})$$

The estimate for the term $W_\alpha \eta$ in (A.17) will be given in few steps. We write $W_\alpha \eta$ as the sum of four terms

$$\begin{aligned}
[W_\alpha \eta](|x|) &= \frac{8\pi i \alpha}{(2\pi)^2 |x|} \int_0^\infty d|y| \frac{g(|y|)}{|y|} \int_0^\infty ds e^{-is|x|} \sin s|y| e^{i\frac{|y|^2}{4\tau}} \times \\
&\times \left[\frac{e^{-i\frac{|y|^2}{4\tau}} - 1}{4\pi\alpha + is} + \frac{1 - e^{-i\frac{|x|^2}{4\tau}}}{4\pi\alpha + is} + e^{-i\frac{|x|^2}{4\tau}} \left(\frac{1}{4\pi\alpha + is} - \frac{1}{4\pi\alpha + is + i\frac{|x|}{2\tau}} \right) + \right. \\
&\quad \left. - e^{-i\frac{|x|^2}{4\tau}} \left(\sqrt{-i\pi\tau} e^{z^2} \operatorname{erfc}(z) - \frac{1}{4\pi\alpha + is + i\frac{|x|}{2\tau}} \right) \right]
\end{aligned} \tag{A.21}$$

We have then

$$\|W_\alpha \eta\|_{L^2(\mathbb{R}^3)}^2 \leq W_1 + W_2 + W_3 + W_4 \tag{A.22}$$

with

$$W_1 = D \int_0^\infty d|x| \left| \int_0^\infty ds \frac{e^{-is|x|}}{4\pi\alpha + is} \mathcal{S} \left(\frac{g(|y|)}{|y|} \left(1 - e^{i\frac{|y|^2}{4\tau}} \right), |y| \right) (s) \right|^2 \tag{A.23}$$

$$W_2 = 2D \int_0^\infty d|x| \left(1 - \cos \frac{|x|^2}{4\tau} \right) \left| \int_0^\infty ds \frac{e^{-is|x|}}{4\pi\alpha + is} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \tag{A.24}$$

$$W_3 = \frac{D}{4\tau^2} \int_0^\infty d|x| |x|^2 \left| \int_0^\infty ds \frac{e^{-is|x|}}{(4\pi\alpha + is)(4\pi\alpha + is + i\frac{|x|}{2\tau})} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \tag{A.25}$$

$$\begin{aligned}
W_4 &= D \int_0^\infty d|x| \left| \int_0^\infty ds e^{-is|x|} \left(\sqrt{-i\pi\tau} e^{z^2} \operatorname{erfc}(z) - \frac{1}{4\pi\alpha + is + i\frac{|x|}{2\tau}} \right) \times \right. \\
&\quad \left. \times \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2
\end{aligned} \tag{A.26}$$

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

$$h(s) = \begin{cases} \frac{1}{4\pi\alpha + is} \mathcal{S} \left(\frac{g(|y|)}{|y|} \left(1 - e^{i\frac{|y|^2}{4\tau}} \right), |y| \right) (s) & s \geq 0 \\ 0 & s < 0 \end{cases} \tag{A.27}$$

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

$$W_1 \leq \frac{D_1}{\tau^2} \int_0^\infty |g(|y|)|^2 |y|^2 d|y| \quad (\text{A.28})$$

It is easily seen from the definition of W_2 that

$$W_2 = 2D \int_0^\infty d|x| \frac{1 - \cos \frac{|x|^2}{4\tau}}{(1 + |x|^2)^2} \left| \int_0^\infty ds \frac{(1 - \frac{d^2}{ds^2}) e^{-is|x|}}{4\pi\alpha + is} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \quad (\text{A.29})$$

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

$$W_2 \leq \frac{D}{\tau^{\frac{3}{2}}} \left\{ \frac{1}{(4\pi\alpha)^2} \int_0^\infty d|y| |g(|y|)|^2 + \int_0^\infty ds \left| \left(1 - \frac{d^2}{ds^2}\right) \frac{\mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s)}{(4\pi\alpha + is)} \right|^2 \right\} \quad (\text{A.30})$$

We rewrite W_3 in the following way

$$W_3 = \frac{D}{4\tau^2} \int_0^\infty d|x| \left| \frac{|x|}{1 + |x|^2} \right|^2 \left| \int_0^\infty ds \frac{(1 - \frac{d^2}{ds^2}) e^{-is|x|}}{(4\pi\alpha + is)(4\pi\alpha + is + i\frac{|x|}{2\tau})} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \quad (\text{A.31})$$

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

$$W_3 \leq \frac{D}{\tau^2} \left\{ \frac{1}{(4\pi\alpha)^4} \int_0^\infty d|y| |g(|y|)|^2 + \int_0^\infty ds \left| \left(1 - \frac{d^2}{ds^2}\right) \frac{\mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s)}{(4\pi\alpha + is)^2} \right|^2 \right\} \quad (\text{A.32})$$

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

$$\left| \frac{d^m}{dz^m} \left(e^{z^2} \operatorname{erfc}(z) - \frac{1}{\sqrt{\pi}z} \right) \right| \leq \left| \frac{1}{\sqrt{\pi}z^{3+m}} \right| \quad \text{for } |z| \rightarrow \infty \quad (\text{A.33})$$

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

$$W_4 \leq \frac{D}{\tau^2} \int_0^\infty d|x| \frac{1}{1 + |x|^2} \int_0^\infty ds \left| \left(1 - \frac{d}{ds}\right) \frac{1}{(4\pi\alpha + is + i\frac{|x|}{2\tau})^3} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \quad (\text{A.34})$$

With the same estimate used in (A.31) it is easily seen that

$$W_4 \leq \frac{\pi D}{2\tau^2} \int_0^\infty ds \left| \left(1 - \frac{d}{ds}\right) \frac{1}{(4\pi\alpha + is)^3} \mathcal{S} \left(\frac{g(|y|)}{|y|} e^{i\frac{|y|^2}{4\tau}}, |y| \right) (s) \right|^2 \quad (\text{A.35})$$

Notice that if $\eta \in L^2_2(\mathbb{R}^3)$ all the integrals in the (A.20), (A.28), (A.30), (A.32), (A.35) are finite and we get estimate (A.12) .

From (A.10) and (A.11) 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

$$\|\Omega_+^{-1}\chi_x\|_{L^2_2(\mathbb{R}^3)} \leq C'(1 + |x|^2)^{\frac{1}{2}} \quad (\text{A.36})$$

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 $\Omega_+^{-1}\chi_x$. \square

To conclude the proof of theorem 4.0.1 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 $\frac{1}{1+\varepsilon}H_0 \otimes \frac{1+\varepsilon}{\varepsilon}H_0$ approximate at the order ε the dynamics of the initial state $\varphi(R)[(\Omega_+^R)^{-1}\chi](r)$ generated by the Hamiltonian H_0^ε .

Using the identity

$$e^{-i\frac{t}{1+\varepsilon}H_0} \left(\frac{\varepsilon(r - r') + (R - R')}{1 + \varepsilon} \right) e^{-i\frac{1+\varepsilon}{\varepsilon}tH_0}(r - r' - (R - R')) = e^{-itH_0}(R - R') e^{-i\frac{t}{\varepsilon}H_0}(r - r') \quad (\text{A.37})$$

we obtain

$$\begin{aligned} \Psi_2^\varepsilon(t; r, R) &= \int_{\mathbb{R}^6} dr' dR' e^{-itH_0}(R - R') e^{-i\frac{t}{\varepsilon}H_0}(r - r') \times \\ &\quad \times \varphi \left(\frac{\varepsilon r' + R'}{1 + \varepsilon} \right) \left[\Omega_+^{-1}\chi \left(\frac{\varepsilon r' + R'}{1 + \varepsilon} + \cdot \right) \right] (r' - R') \end{aligned} \quad (\text{A.38})$$

We prove the last lemma

Lemma 1. *There exists a constant $C_3 > 0$ such that for any $t \in \mathbb{R}$ one has*

$$\|\Psi_2^\varepsilon(t) - \Psi^a(t)\| \leq C_3\varepsilon \quad (\text{A.39})$$

Proof. Given the unitarity of the free propagator

$$\begin{aligned} \|\Psi_2^\varepsilon(t) - \Psi^a(t)\|^2 &= \int_{\mathbb{R}^6} dR dr \left| \varphi\left(\frac{\varepsilon r + R}{1 + \varepsilon}\right) \left[\Omega_+^{-1} \chi\left(\frac{\varepsilon r + R}{1 + \varepsilon} + \cdot\right) \right] (r - R) + \right. \\ &\quad \left. - \varphi(R) \left[\Omega_+^{-1} \chi(R + \cdot) \right] (r - R) \right|^2 \end{aligned} \quad (\text{A.40})$$

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

$$\begin{aligned} \|\Psi_2^\varepsilon(t) - \Psi^a(t)\|^2 &= \int_{\mathbb{R}^6} dx dy \left| \varphi(x) \left[\Omega_+^{-1} \chi(x + \cdot) \right] (y) + \right. \\ &\quad \left. - \varphi\left(x - \frac{\varepsilon}{1 + \varepsilon} y\right) \left[\Omega_+^{-1} \chi\left(x - \frac{\varepsilon}{1 + \varepsilon} y + \cdot\right) \right] (y) \right|^2 \end{aligned} \quad (\text{A.41})$$

In the limit of small ε we can write

$$\begin{aligned} \|\Psi_2^\varepsilon(t) - \Psi^a(t)\|^2 &\leq \varepsilon^2 \int_{\mathbb{R}^6} dx dy |y|^2 |\nabla_x [\varphi(x) \Omega_+^{-1} \chi_x(y)]|^2 \\ &\leq \varepsilon^2 ((\diamond 1) + (\diamond 2)) \end{aligned} \quad (\text{A.42})$$

Let us prove that the terms $(\diamond 1)$, $(\diamond 2)$ in (A.42) are finite. Using the definition (3.30) of Ω_+^{-1} and the explicit form of the generalized functions $\Phi_+(x, k)$ we obtain

$$\begin{aligned} (\diamond 1) &= \int_{\mathbb{R}^6} dx dy |\nabla_x \varphi(x)|^2 |y|^2 |\Omega_+^{-1} \chi_x(y)|^2 = \\ &= \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^6} dx dk |\nabla_x \varphi(x)|^2 \left| \nabla_k \int_{\mathbb{R}^3} dz \left(e^{-ikz} + \frac{1}{4\pi\alpha - i|k|} \frac{e^{i|k||z|}}{|z|} \right) \chi_x(z) \right|^2 \leq \\ &\leq (\diamond 3) + (\diamond 4) \end{aligned} \quad (\text{A.43})$$

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

$$\begin{aligned} (\diamond 3) &= \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx |\nabla_x \varphi(x)|^2 \int_{\mathbb{R}^3} dz ||z| \chi_x(z)|^2 \leq \\ &\leq \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx |\nabla_x \varphi(x)|^2 \int_{\mathbb{R}^3} dz ||z| \chi_x(z)| + \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}^3} dx |\nabla_x \varphi(x)|^2 |x|^2 \|\chi(z)\|_{L^2(\mathbb{R}^3)}^2 \end{aligned} \quad (\text{A.44})$$

For the term $(\diamond 4)$ we have

$$(\diamond 4) = \left(\frac{1}{2\pi} \right)^3 \int_{\mathbb{R}^6} dx dk |\nabla_x \varphi(x)|^2 \left| \frac{d}{d|k|} \int_{\mathbb{R}^3} dz \frac{1}{4\pi\alpha - i|k|} \frac{e^{i|k||z|}}{|z|} \chi_x(z) \right|^2 \leq (\diamond 5) + (\diamond 6) \quad (\text{A.45})$$

with

$$(\diamond 5) = \int_{\mathbb{R}^6} dx dk \frac{|\nabla_x \varphi(x)|^2}{((4\pi\alpha)^2 + |k|^2)^2} \left| \int_{\mathbb{R}^3} dz \frac{e^{i|k||z|}}{|z|} \chi_x(z) \right|^2 \quad (\text{A.46})$$

In (A.46) the only problem is represented by the integral in the variable z . Making explicit the x dependence of $\chi_x(z)$ we have

$$\begin{aligned} \left| \int_{\mathbb{R}^3} dz \frac{e^{i|k||z|}}{|z|} \chi(z+x) \right|^2 &= \left| \int_{\mathbb{R}^3} d\xi \frac{e^{i|k||\xi-x|}}{|\xi-x|(1+|\xi|^2)^{\frac{1}{2}}} \chi(\xi) (1+|\xi|^2)^{\frac{1}{2}} \right|^2 \leq \\ &\leq \left(\int_{\mathbb{R}^3} d\xi |\chi(\xi)|^2 (1+|\xi|^2) \right) \left(\int_{\mathbb{R}^3} d\xi \frac{1}{|\xi-x|^2 (1+|\xi|^2)} \right) = \\ &= \|(1+|\cdot|^2)^{\frac{1}{2}} \chi\|_{L^2(\mathbb{R}^3)}^2 \left\| \frac{1}{|\cdot|(1+|\cdot+x|^2)^{\frac{1}{2}}} \right\|_{L^2(\mathbb{R}^3)}^2 \end{aligned} \quad (\text{A.47})$$

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

$$\left\| \frac{1}{|\cdot|(1+|\cdot+x|^2)^{\frac{1}{2}}} \right\|_{L^2(\mathbb{R}^3)}^2 \leq \frac{\pi^2}{|x|} \quad (\text{A.48})$$

We finally estimate the term

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

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

$$\begin{aligned} \left| \int_{\mathbb{R}^3} dz \chi(z+x) e^{i|k||z|} \right|^2 &= \left| \int_{\mathbb{R}^3} d\xi \chi(\xi) e^{i|k||\xi-x|} \right|^2 = \left| \int_{\mathbb{R}^3} d\xi \chi(\xi) \frac{-i}{|k|} \frac{\xi-x}{|\xi-x|} \nabla_\xi e^{i|k||\xi-x|} \right|^2 \leq \\ &\leq \frac{1}{|k|^2} \int_{\mathbb{R}^3} d\xi |\nabla_\xi \chi(\xi)|^2 + \frac{4}{|k|^2} \left| \int_{\mathbb{R}^3} d\xi \frac{e^{i|k||\xi-x|}}{|\xi-x|} \chi(\xi) \right|^2 \end{aligned} \quad (\text{A.50})$$

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

$$(\diamond 2) = \int_{\mathbb{R}^6} dx dy |\varphi(x)|^2 |y|^2 |\nabla_x \Omega_+^{-1} \chi_x(y)|^2 \quad (\text{A.51})$$

is finite. Notice that

$$|\nabla_x \Omega_+^{-1} \chi_x(y)|^2 = \sum_{i=1}^3 |\partial_{x_i} (\Omega_+^{-1} \chi_x)(y)|^2 = \sum_{i=1}^3 |\Omega_+^{-1} f_{i,x}(y)|^2 \quad (\text{A.52})$$

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 $(\diamond 2)$ can be obtained with the same procedure used for $(\diamond 1)$, 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 A is satisfied. \square

Appendix B

The modified Krein Formula

In this appendix is given a short introduction to the most general expression of the Krein-Naimark formula following the works of S.Albeverio and K.Pankrashkin [11]. This formula provides a parametrization of all selfadjoint extensions of a symmetric operator, involving in the simplest way global parameters, as the boundary conditions, connected to the spectral properties of the selfadjoint extensions.

Let S be a closed densely defined symmetric operator with deficiency indices (n, n) , $0 < n \leq \infty$, acting on a Hilbert space \mathcal{H} . Consider now an auxiliary Hilbert space \mathcal{G} such that $\dim \mathcal{G} = n$.

We introduce the definition of *boundary triple* $\Pi = \{\mathcal{G}, \Gamma_1, \Gamma_2\}$, where Γ_1 and Γ_2 are linear maps from the domain $\text{dom } S^*$ of the adjoint of S to \mathcal{G} and the following two conditions are satisfied:

- a generalized Green identity

$$\langle \phi, S^* \psi \rangle - \langle S^* \phi, \psi \rangle = \langle \Gamma_1 \phi, \Gamma_2 \psi \rangle - \langle \Gamma_2 \phi, \Gamma_1 \psi \rangle \quad (\text{B.1})$$

- the map $(\Gamma_1, \Gamma_2) : \text{dom } S^* \rightarrow \mathcal{G} \oplus \mathcal{G}$ is surjective

While it is well known that the self-adjoint extensions are parametrized by self-adjoint linear relation in $\mathcal{G} \otimes \mathcal{G}$ in many situations it can be more useful to parametrize them with boundary conditions. Boundary conditions will take the form the form $A\Gamma_1\phi = B\Gamma_2\phi$ (where A and B are bounded linear operator acting on \mathcal{G}).

We want to write a formula for the resolvent in term of A and B that permits to characterize the whole family of self-adjoint extensions of S

B.1 Parameterization of self-adjoint relations

We will need some notion from the theory of linear relations. Any linear subspace of $\mathcal{G} \oplus \mathcal{G}$ defines a linear relation on \mathcal{G} . We recall briefly some usual definitions for a linear relation Λ :

- the *domain* $\text{dom}\Lambda = \{x \in \mathcal{G} : \exists y \in \mathcal{G} \text{ with } (x, y) \in \Lambda\}$
- the *range* $\text{ran}\Lambda = \{x \in \mathcal{G} : \exists y \in \mathcal{G} \text{ with } (y, x) \in \Lambda\}$
- the *kernel* $\text{ker}\Lambda = \{x \in \mathcal{G} : (x, 0) \in \Lambda\}$

We can define the linear relations:

- the *inverse* $\Lambda^{-1} = \{(x, y) : (y, x) \in \Lambda\}$
- the *adjoint* $\Lambda^* = \{(x_1, x_2) : \langle x_1, y_2 \rangle = \langle x_2, y_1 \rangle\}$

The graph of any linear operator L on \mathcal{G} is a linear relation, which will be denoted by $\text{gr } L$. Clearly, if L is invertible, then $\text{gr } L^{-1} = (\text{gr } L)^{-1}$. For arbitrary linear operators L', L'' one has $\text{gr } L' + \text{gr } L'' = \text{gr } (L' + L'')$. Therefore, the set of linear operators is naturally embedded into the set of linear relations. In what follows we consider mostly only closed linear relations, i.e. which are closed linear subspaces in $\mathcal{G} \oplus \mathcal{G}$. Clearly, this notion generalizes the notion of a closed operator.

In analogy with operators, can be introduced the notions of the *resolvent set* $\text{res } \Lambda$ of a closed linear relation Λ by the rule $\text{res } \Lambda = \{\lambda \in \mathbb{C} : \text{ker}(\Lambda - \lambda I) = 0 \text{ and } \text{ran}(\Lambda - \lambda I) = \mathcal{G}\}$, where $I \equiv \text{gr id}_{\mathcal{G}} = \{(x, x), x \in \mathcal{G}\}$. In other words, the condition $\lambda \in \text{res } \Lambda$ means that $(\Lambda - \lambda I)^{-1}$ is the graph of a certain linear operator defined everywhere; this operator is bounded due to the closed graph theorem.

A linear relation Λ on \mathcal{G} is called *symmetric* if $\Lambda \subset \Lambda^*$ and is called *self-adjoint* if $\Lambda = \Lambda^*$. A linear operator L in \mathcal{G} is symmetric (respectively, self-adjoint), iff its graph is a symmetric (respectively, self-adjoint) linear relation. A self-adjoint linear relation (abbreviated as s.a.l.r.) is always maximal symmetric, but the converse is not true; examples are given by the graphs of maximal symmetric operators with deficiency indices $(m, 0)$, $m > 0$.

The self adjoint linear relations can be presented using two bounded linear operators on \mathcal{G} , called A and B . We introduce the notation

$$\Lambda^{A,B} = \{(x_1, x_2) \in \mathcal{G} \oplus \mathcal{G}, \quad Ax_1 = Bx_2\}.$$

We say that a linear relation Λ is *parameterized by the operators A and B* if $\Lambda = \Lambda^{A,B}$. Conditions for $\Lambda^{A,B}$ to be self-adjoint can be written in many ways, see e.g. [22, 36, 78].

Proposition 2 (Proposition B in [22]). *Denote by $M^{A,B}$ an operator acting on $\mathcal{G} \oplus \mathcal{G}$ by the rule*

$$M^{A,B} = \begin{pmatrix} A & -B \\ B & A \end{pmatrix}, \quad (\text{B.2})$$

then the linear relation $\Lambda^{A,B}$ is self-adjoint iff A and B satisfy the following two conditions:

$$AB^* = BA^*, \quad (\text{B.3})$$

$$\ker M^{A,B} = 0. \quad (\text{B.4})$$

Proposition 3 (Theorem 3.1.4 in [48]). *For a given linear relation Λ in \mathcal{G} there is a unique unitary operator U in \mathcal{G} (called the Cayley transform of Λ) such that the condition $(x_1, x_2) \in \Lambda$ is equivalent to $i(1+U)x_1 = (1-U)x_2$, i.e. $\Lambda = \Lambda^{i(1+U), 1-U}$.*

Taking U in the form $U = e^{-2i\Phi}$, where Φ is a self-adjoint operator in \mathcal{G} , one write any s.a.l.r. as $\Lambda^{\cos \Phi, \sin \Phi}$.

Although proposition 3 claims that there exists a one-to-one correspondence between s.a.l.r.s and unitary operators, for a given s.a.l.r. Λ it is difficult to find its Cayley transform, but there are many other ways to represent it as $\Lambda^{A,B}$ with suitable A and B .

In what follows we will need a parameterization of s.a.l.r. satisfying stronger conditions than (B.3) and (B.4). More precisely, we replace the condition (B.4) by

$$0 \in \text{res } M^{A,B}. \quad (\text{B.5})$$

We say that a pair of bounded operators A and B satisfying (B.3) and (B.4) is *normalized* if the condition (B.5) is satisfied. Clearly, in the case of finite-dimensional \mathcal{G} the conditions (B.4) and (B.5) are equivalent. Moreover, in this case these conditions are equivalent to the following one [60]:

the $n \times 2n$ matrix (AB) has maximal rank.

(Note that this can be written also as $\det(AA^* + BB^*) \neq 0$, which can be found in the textbooks on operator theory [6, Section 125, Theorem 4]). In general, the conditions (B.4) and (B.5) do not coincide: if one replaces A by LA and B by LB , where L is a bounded linear operators with the subspace $\Lambda^{A,B}$, but the condition (B.5) will not be satisfied. Moreover, this construction is the only source of “denormalization”.

Proposition 4. *Let A, B, C, D be bounded operators in \mathcal{G} and Λ be a s.a.l.r. in \mathcal{G} such that $\Lambda = \Lambda^{A,B} = \Lambda^{C,D}$. Assume that A and B are normalized, then there exists a bounded injective operator L on \mathcal{H} with $C = LA$ and $D = LB$.*

Proof. Introduce operators $M_1, M_2 : \mathcal{G} \oplus \mathcal{G} \rightarrow \mathcal{G}$ by $M_1(x_1, x_2) = Ax_1 - Bx_2$, $M_2(x_1, x_2) = Cx_1 - Dx_2$, $x_1, x_2 \in \mathcal{G}$. The condition (B.5) says, in particular, that $\text{ran } M_1 = \mathcal{G}$. Clearly, the null spaces of M_1 and M_2 coincide, $\ker M_1 = \ker M_2 = \Lambda$, therefore, there exists an injective operator L in \mathcal{H} such that $M_2 = LM_1$, which implies $C = LA$ and $D = LB$. Let us show that L is bounded. Use the notation (B.2), then there holds $M^{C,D} = (L \oplus L)M^{A,B}$. Due to the

condition (B.5) the operator $M^{A,B}$ has a bounded inverse defined everywhere. Therefore, $L \oplus L = M^{C,D}(M^{A,B})^{-1}$ is bounded and defined everywhere, so is L . \square

It is important to emphasize that for a given s.a.l.r one can always find a normalized parameterization, as the following proposition shows.

Proposition 5. (a) *Let U be a unitary operator in \mathcal{G} , then the operators $A = i(1 + U)$ and $B = 1 - U$ satisfy the conditions (B.3) and (B.5).*

(b) *Any s.a.l.r. can be parameterized by operators A and B satisfying (B.3) and (B.5).*

Proof. (a) The condition (B.3) is obviously satisfied, so we prove only (B.5). First of all note that the operator M^* adjoint to $M = M^{A,B}$ is given by the following operator-matrix:

$$M^* = \begin{pmatrix} A^* & B^* \\ -B^* & A^* \end{pmatrix}$$

or, in our case,

$$M^* = \begin{pmatrix} -i(1 + U^*) & 1 - U^* \\ U^* - 1 & -i(1 + U^*) \end{pmatrix}.$$

Let us show that $\ker M^* = 0$. Assume $x = (x_1, x_2) \in \ker M^*$, $x_1, x_2 \in \mathcal{G}$, then

$$-i(1 + U^*)x_1 + (1 - U^*)x_2 = 0, \quad (\text{B.6})$$

$$(U^* - 1)x_1 - i(1 + U^*)x_2 = 0. \quad (\text{B.7})$$

Multiplying (B.6) by i and adding the result to (B.7) one arrives at $U^*(x_1 - ix_2) = 0$; as U^* is unitary, we have $x_1 - ix_2 = 0$. On the other hand, multiplying (B.6) by i again and subtracting (B.7) from it, we obtain $x + ix_2 = 0$, which says that $x_1 = x_2 = 0$.

As $(\text{ran } M)^\perp = \ker M^*$, the linear subspace $\text{ran } M$ is dense in \mathcal{G} . Now to prove (B.5) it is sufficient to show that for any sequence $(x^n) \in \mathcal{G} \oplus \mathcal{G}$, $x^n = (x_1^n, x_2^n)$, $x_1^n, x_2^n \in \mathcal{G}$, the condition $\lim_{n \rightarrow \infty} Mx^n = 0$ implies the convergence of (x^n) to 0, which we will do now.

Assuming the existence of the limits

$$\lim_{n \rightarrow \infty} (i(1 + U)x_1^n + (U - 1)x_2^n) = 0, \quad \lim_{n \rightarrow \infty} ((1 - U)x_1^n + i(1 + U)x_2^n) = 0$$

one sees immediately that the sequences $(x_1^n + ix_2^n)$ and $(U(-x_1^n + ix_2^n))$ converge to 0. As U is unitary, the sequence $(-x_1^n + ix_2^n)$ converges to 0 too, which shows that $\lim_{n \rightarrow \infty} x_1^n = \lim_{n \rightarrow \infty} x_2^n = 0$.

(b) This is an obvious corollary of (a) and proposition 3. \square

Finally, we are able to give another description of a s.a.l.r. with the help of its normalized parameterization.

Lemma 2. *Let bounded operators A, B parameterize a s.a.l.r. in \mathcal{G} and be normalized, then $\Lambda^{A,B} = \{(B^*u, A^*u), u \in \mathcal{G}\}$.*

Proof. Set $\Lambda' := \{(B^*u, A^*u), u \in \mathcal{G}\}$. Clearly, due to (B.3) there holds the inclusion $\Lambda' \subset \Lambda^{A,B}$. Let us show that $\Lambda^{A,B} = \Lambda'$. The condition (B.5) means, in particular, that the operator $(M^{A,B})^*$ has a bounded inverse and, therefore, maps closed sets to closed sets. As $\Lambda' = (M^{A,B})^*(0 \oplus \mathcal{G})$, Λ' is closed. As $\Lambda^{A,B}$ is also closed, it is sufficient to prove that $(\Lambda')^\perp \cap \Lambda^{A,B} = 0$. Assume $x = (x_1, x_2) \in (\Lambda')^\perp \cap \Lambda^{A,B}$, $x_1, x_2 \in \mathcal{G}$. The condition $x \in \Lambda^{A,B}$ means that $Ax_1 - Bx_2 = 0$, and the equality $\langle x, y \rangle = 0$ for any $y \in \Lambda'$ results in $\langle x_1, B^*u \rangle + \langle x_2, A^*u \rangle = 0$ or $\langle Bx_1 + Ax_2, u \rangle = 0$ for any $u \in \mathcal{G}$, i.e. $Bx_1 + Ax_2 = 0$. Therefore, $M^{A,B}x = 0$ and due to (B.5) there holds $x = 0$. \square

B.2 Resolvents of self-adjoint extensions

The language of linear relations is widely used in the theory of self-adjoint extensions of symmetric operators [48, 59, 78]. We point out that any symmetric operator with equal deficiency indices (finite or infinite) has a boundary triple [48, Theorem 3.1.5].

Proposition 6 (Theorem 3.1.6 in [48]). *Let S be a closed symmetric operator with equal deficiency indices acting on a certain Hilbert space, and $(\mathcal{G}, \Gamma_1, \Gamma_2)$ be its boundary triple, then there is a bijection between all self-adjoint extensions of S and s.a.l.r.'s on \mathcal{G} . A self-adjoint extension H^Λ corresponding to a s.a.l.r. Λ is the restriction of S^* to elements $\phi \in \text{dom } S^*$ satisfying the abstract boundary conditions $(\Gamma_1\phi, \Gamma_2\phi) \in \Lambda$.*

To investigate spectral properties of the self-adjoint extensions it is useful to know their resolvents. To write Krein's formula for the resolvents we need some additional constructions [35]. For $z \in \mathbb{C} \setminus \mathcal{R}$, let \mathcal{N}_z denote the corresponding deficiency subspace for S , i.e. $\mathcal{N}_z = \ker(S^* - z)$. The restrictions of Γ_1 and Γ_2 onto \mathcal{N}_z are invertible linear maps from \mathcal{N}_z to \mathcal{G} . Put $\gamma(z) = (\Gamma_1|_{\mathcal{N}_z})^{-1}$ and $Q(z) = \Gamma_2\gamma(z)$; these maps form holomorphic families from $\mathbb{C} \setminus \mathcal{R}$ to the spaces $\mathcal{L}(\mathcal{G}, \mathcal{H})$ and $\mathcal{L}(\mathcal{G}, \mathcal{G})$ of bounded linear operators from \mathcal{G} to \mathcal{H} and from \mathcal{G} to \mathcal{G} respectively. Denote by H^0 the self-adjoint extension of S given by the boundary condition $\Gamma_1\phi = 0$, then the maps $\gamma(z)$ and $Q(z)$ have analytic continuations to the resolvent set $\text{res } H^0$, and for all $z, \zeta \in \text{res } H^0$ one has, in particular,

$$Q(z) - Q^*(\zeta) = (z - \bar{\zeta}) \gamma^*(\zeta) \gamma(z). \quad (\text{B.8})$$

The maps $\gamma(z)$ and $Q(z)$ are called the Γ -field and the Q -function for the pair (S, H^0) , respectively [44, 62, 64]. (The Q -function is called sometimes the *Weyl M -function* of the boundary triple $(\mathcal{G}, \Gamma_1, \Gamma_2)$ [8, 25, 35].) Similar objects arise naturally also in the study of singular perturbations of self-adjoint operators [73, 74].

The following proposition describes the resolvents of the self-adjoint extensions of S .

Proposition 7 (Krein's resolvent formula, cf. Propositions 1 and 2 in [35]). *Let H^Λ be a self-adjoint extension of S , which is the restriction of S^* to the set of functions $\phi \in \text{dom } S^*$ satisfying $(\Gamma_1\phi, \Gamma_2\phi) \in \Lambda$, where Λ is a s.a.l.r. in \mathcal{G} . Then a number $z \in \text{res } H^0$ lies in the spectrum of H^Λ iff $0 \notin \text{res } (\text{gr } Q(z) - \Lambda)^{-1}$. For any $z \in \text{res } H^0 \cap \text{res } H^\Lambda$ there holds*

$$(H^\Lambda - z)^{-1} = (H^0 - z)^{-1} - \gamma(z) C_\Lambda(z) \gamma^*(\bar{z}), \quad (\text{B.9})$$

where $C_\Lambda(z)$ is a bounded linear operator on \mathcal{G} with $\text{gr } C_\Lambda(z) = (\text{gr } Q(z) - \Lambda)^{-1}$.

It is worth emphasizing that the correspondence between the spectral types of H^Λ and $C_\Lambda(z)$ (discrete spectra, essential spectra etc.) is a rather difficult problem, cf. [8, 20, 25]

The calculation of $C_\Lambda(z)$ is a rather difficult technical problem, as it involves "generalized" operations with linear relations. Such difficulties do not arise if Λ is the graph of a certain self-adjoint linear operator L (i.e. if Λ can be injectively projected onto $\mathcal{G} \oplus 0$); the boundary conditions take the form $\Gamma_2\phi = L\Gamma_1\phi$, and such extensions are called *disjoint to H^0* because of the equality $\text{dom } H^\Lambda \cap \text{dom } H^0 = \text{dom } S$ (the operator S is then called the *maximal common part* of H^0 and H^Λ). Then the subspace $\text{gr } Q(z) - \Lambda$ is the graph of the invertible operator $Q(z) - L$, and $C^\Lambda(z) = (Q(z) - L)^{-1}$.

As we have shown in proposition 5, all self-adjoint boundary conditions can be represented with the help of two bounded linear operators A and B by

$$A\Gamma_1\phi = B\Gamma_2\phi \quad \Leftrightarrow \quad (\Gamma_1\phi, \Gamma_2\phi) \in \Lambda^{A,B}, \quad (\text{B.10})$$

where A and B satisfy (B.3) and (B.5). Our aim is to show that the resolvent formula (B.9) admits a simple form in terms of these two operators.

Lemma 3. *Let bounded operators A, B parameterize a s.a.l.r. in \mathcal{G} and be normalized. Then for any $z \in \text{res } H^0$ the following three conditions are equivalent:*

- (a) $0 \in \text{res } (\text{gr } Q(z) - \Lambda^{A,B})$,
- (b) $0 \in \text{res } (BQ(z) - A)$,
- (c) $0 \in \text{res } (Q(z)B^* - A^*)$.

If these conditions are satisfied, then

$$(\text{gr } Q(z) - \Lambda^{A,B})^{-1} = \text{gr } B^*(Q(z)B^* - A^*)^{-1} = \text{gr } (BQ(z) - A)^{-1}B. \quad (\text{B.11})$$

Proof. Let us express the linear relation $\text{gr } Q(z) - \Lambda^{A,B}$ through A and B . Due to lemma 2 one has $\Lambda^{A,B} = \{(B^*u, A^*u), u \in \mathcal{G}\}$. Therefore, $\text{dom}(\text{gr } Q(z) - \Lambda^{A,B}) = \text{ran } B^*$, and there holds

$$(\text{gr } Q(z) - \Lambda^{A,B}) = \left\{ (B^*u, Q(z)B^*u - A^*u), u \in \mathcal{G} \right\}. \quad (\text{B.12})$$

Assume that (a) is satisfied and show (c). Clearly, $\text{ran}(\text{gr } Q(z) - \Lambda^{A,B}) = \text{ran}(Q(z)B^* - A^*)$, and there holds $\text{ran}(Q(z)B^* - A^*) = \mathcal{G}$. We show now that $\ker(Q(z)B^* - A^*) = 0$. Let $(Q(z)B^* - A^*)u = 0, u \in \mathcal{G}$. As $\ker(\text{gr } Q(z) - \Lambda^{A,B}) = 0$, the corresponding first component in $(B^*u, (Q(z)B^* - A^*)u)$ must vanish, i.e. $B^*u = 0$, and then $A^*u = 0$. But $\ker A^* \cap \ker B^* = 0$ due to (B.5), and $u = 0$. Therefore, the operator $Q(z)B^* - A^*$ has a bounded inverse due to the closed graph theorem. Hence (a) implies (c).

Now let (c) hold, then we can rewrite (B.12)

$$\text{gr } Q(z) - \Lambda^{A,B} = \left\{ (B^*(Q(z)B^* - A^*)^{-1}x, x), x \in \mathcal{G} \right\}, \quad (\text{B.13})$$

and we get immediately $\text{ran}(Q(z) - \Lambda^{A,B}) = \mathcal{G}$ and $\ker(Q(z) - \Lambda^{A,B}) = 0$, which exactly (a). Therefore, we have shown that (a) is equivalent to (c).

Note that the condition (a) and, therefore, also (c), is invariant under the change $z \leftrightarrow \bar{z}$, because they define the resolvent set of the self-adjoint operator $H^{A,B}$, and the resolvent set is symmetric under the complex conjugation. The equivalence of (b) and (c) follows from the fact that $Q(\bar{z})B^* - A^*$ has 0 in the resolvent set if and only if its adjoint $BQ(z) - A$ has the same property (here one can use the equality $Q(\bar{z}) = Q^*(z)$ following from (B.8)).

We have already proved the first equality in (B.12), see (B.13). Let us show the second one. Let us use the notation of proposition 7. Replacing z in (B.9) by \bar{z} and taking the adjoint on the both sides one sees immediately that $C_\Lambda^*(\bar{z}) = C_\Lambda(z)$ for any $z \in \text{res } H^0$. On the other hand, we have shown already that for $\Lambda = \Lambda^{A,B}$ one has $C_\Lambda(z) = B^*(Q(z)B^* - A^*)^{-1}$, therefore, $(BQ(z) - A)^{-1}B = C_\Lambda^*(\bar{z}) = C_\Lambda(z) = B^*(Q(z)B^* - A^*)^{-1}$. \square

Now we are in position to reformulate proposition 7 completely in the operator language, without using linear relations.

Theorem B.2.1 (Resolvent formula for normalized parameters). *Let $H^{A,B}$ be the self-adjoint extension of S corresponding to the boundary conditions (B.10) with normalized A and B . A number $z \in \text{res } H^0$ lies in $\text{spec } H^{A,B}$ iff $0 \in \text{spec}(BQ(z) - A)$ or, equivalently, $0 \in \text{spec}(Q(z)B^* - A^*)$. For any $z \in \text{res } H^0 \cap \text{res } H^{A,B}$ there holds*

$$(H^{A,B} - z)^{-1} = (H^0 - z)^{-1} - \gamma(z)B^*(Q(z)B^* - A^*)^{-1}\gamma^*(\bar{z}), \quad (\text{B.14})$$

$$(H^{A,B} - z)^{-1} = (H^0 - z)^{-1} - \gamma(z)(BQ(z) - A)^{-1}B\gamma^*(\bar{z}). \quad (\text{B.15})$$

Proof. Follows from lemma 3. □

Note that by setting $A = i(1 + U)$, $B = 1 - U$ one obtains a global expression for the resolvents which covers the whole family of self-adjoint extensions. A finite-dimensional case of this resolvent formula was obtained in [11] in the context of singular quantum-mechanical interactions.

Theorem B.2.2 (Eigenvalues of self-adjoint extensions). *Let $H^{A,B}$ be the self-adjoint extension of S corresponding to the boundary conditions (B.10) with A and B satisfying (B.3) and (B.4). The value $z \in \text{res } H^0$ is an eigenvalue of $H^{A,B}$ iff $\ker(BQ(z) - A) \neq 0$, and in this case one has $\ker(H^{A,B} - z) = \gamma(z) \ker(BQ(z) - A)$.*

Proof. Let us show first that $\gamma(z) \ker(BQ(z) - A) \subset \ker(H^{A,B} - z)$. For any $\xi \in \ker(BQ(z) - A)$ the element $f(z, \xi) := \gamma(z)\xi$ is an eigenfunction of S^* with the eigenvalue z , because $\gamma(z)$ is an isomorphism between $\ker(S^* - z)$ and \mathcal{G} . Moreover, one has $\Gamma_1 f(z, \xi) = \Gamma_1 \Gamma_1^{-1} \xi = \xi$ and $\Gamma_2 f(z, \xi) = \Gamma_2 \gamma(z)\xi = Q(z)\xi$, therefore, $A\Gamma_1 f(z, \xi) - B\Gamma_2 f(z, \xi) = -(BQ(z) - A)\xi = 0$, which means that $f(z, \xi)$ is in the domain of $H^{A,B}$. Therefore, $f(z, \xi)$ is an eigenvector of $H^{A,B}$ with eigenvalue z .

Now let $z \in \text{res } H^0$ be an eigenvalue of $H^{A,B}$ and f be a non-zero element of the corresponding subspace. Then f is also an eigenvector of S^* . As $\gamma(z)$ is an isomorphism between $\ker(S^* - z)$ and \mathcal{G} , there exists $\xi \in \mathcal{G} \setminus \{0\}$ such that $f = \gamma(z)\xi$. As previously, there holds $\Gamma_1 f = \xi$, $\Gamma_2 f = Q(z)\xi$, and the condition $f \in \text{dom } H^{A,B}$ takes the form $A\Gamma_1 f - B\Gamma_2 f \equiv -(BQ(z) - A)\xi = 0$. □

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