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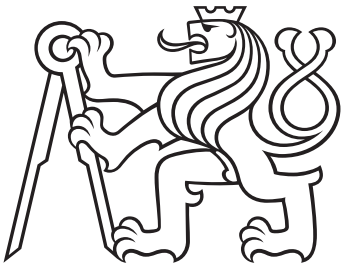

Nonhermitian Quantum Mechanics in Atomic and Laser Physics

Nehermitovská kvantová mechanika v atomové a laserové fyzice

BACHELOR'S DEGREE PROJECT

Author: Jakub Vaniš
Supervisor: RNDr. Milan Šindelka, Ph.D.
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Student: Jakub Vaniš

Studijní program: Aplikace přírodních věd

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Název práce: (česky) Nehermitovská kvantová mechanika v atomové a laserové fyzice

Název práce: (anglicky) Nonhermitian quantum mechanics in atomic and laser physics

Pokyny pro vypracování:

1) Základy kvantové teorie rozptylu, fenomén metastabilních stavů (rezonancí)
2) Nehermitovský popis rezonancí za použití metody komplexního škálování
3) Teorie Siegertových (pseudo)stavů
4) Fenomén nehermitovských degenerací (exceptional points)
5) Nehermitovský popis interakce atomů s laserem
6) Anti-vázané stavy a jejich fyzikální význam

Doporučená literatura:

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V Praze dne 20.10.2021

Author's declaration

I declare that this Bachelor's Degree Project is entirely my own work and I have listed all the used sources in the bibliography.

In Prague on ....

Jakub Vaniš

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I wish to thank my supervisor RNDr. Milan Šindelka, Ph.D. for his invaluable advice and guidance throughout this project.

Jakub Vaniš

Title:
Nonhermitian Quantum Mechanics in Atomic and Laser Physics

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Study Program: Applications of Natural Sciences
Branch of Studies: Mathematical Physics
Type of Work: Bachelor's Degree Project

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Abstract: In this project we explore the field of theoretical physics known as nonhermitian quantum mechanics (NHQM). We discuss an application of NHQM on describing the interaction of atoms with a weak intensity laser and formation of the so-called exceptional point. NHQM is inherently tied to scattering and decay phenomena involving metastable states of quantum systems known as resonances. Unlike conventional hermitian quantum mechanics, NHQM possesses powerful tools to efficiently describe physical processes involving resonances and to predict new phenomena. A simple 1D toy model is used along the way to better illustrate the formalism and to give examples of the application of NHQM methods.

Key words: Nonhermitian Quantum Mechanics, Complex Scaling, Gamow-Siegert States, Floquet Theory, Exceptional Points

Název práce:
Nehermitovská kvantová mechanika v atomové a laserové fyzice

Autor: Jakub Vaniš

Abstrakt: V této práci zkoumáme oblast teoretické fyziky známou jako nehermitovská kvantová mechanika (NHQM) a diskutujeme její aplikaci při popisu interakce atomů s laserem slabé intenzity a vzniku tzv. nehermitovské degenerace. NHQM je inherentně spojena s rozptylovými a rozpadovými jevy zahrnujícími metastabilní stavy kvantových systémů známé jako rezonance. Na rozdíl od konvenční hermitovské kvantové mechaniky, má NHQM výkonné nástroje k efektivnímu popisu fyzikálních procesů zahrnujících rezonance a k předpovědi nových jevů. Pro lepší ilustraci formalismu a pro uvedení příkladů aplikace metod NHQM je použit jednoduchý 1D model.

Klíčová slova: Nehermitovská kvantová mechanika, Komplexní škálování, Gamow-Siegertovy stavy, Floquetova teorie, Nehermitovské degenerace

Contents

Introduction

This Bachelor project focuses on reviewing and exploration of an important and turbulently evolving field of theoretical and mathematical physics called the ***non-hermitian quantum mechanics (NHQM)***. NHQM is inherently associated with scattering and decay phenomena which involve metastable states of quantum systems, the so-called ***resonances***.

Metastable states (resonances) correspond to situations when the studied quantum system (atom, molecule, atomic nucleus) is "almost bound" or "almost stable" yet it has enough energy to decay (disintegrate) into fragments (electrons, ions, photons, products of a chemical reaction, or products of an alpha-decay). Resonances can often be formed by exposing an originally bound system to an external field (electrostatic, magnetostatic, or to an oscillating field of a laser). Due to the just mentioned decay into fragments, metastable systems possess a finite lifetime, as opposed to true bound states, which live infinitely long. Resonances are manifested physically by ***Breit-Wigner*** (Lorentzian) ***peaks*** in the experimentally measurable scattering amplitudes (transmission probabilities, cross sections).

Physical phenomena involving metastable states are very rich but difficult to describe using the conventional framework of the hermitian quantum mechanics (HQM). NHQM offers an extremely powerful alternative. (Yet one needs to keep in mind that NHQM is fully equivalent to HQM when it comes to all the experimentally observable quantities.) As the name already suggests, NHQM is dealing with nonhermitian operators, in contrast to HQM. Correspondingly, the energy eigenvalues of a nonhermitian Hamiltonian are complex valued, such that the resonances acquire a negative imaginary part proportional to their inverse lifetime (see Chapters 2-3 for a self contained treatment of this issue). NHQM even enables to predict physical phenomena whose existence one can hardly anticipate when working within the standard HQM (in particular, an emergence of the so-called exceptional points and their physical fingerprints, see Chapters 2-3 for details).

The purpose of this project is to review the formalism of NHQM and to discuss one of its important applications: an ***interaction of atoms with a weak intensity laser*** and formation of the so-called ***exceptional point*** by the laser. The structure of the project is as follows:

In **Chapter 1** we outline the basic notions of hermitian scattering theory. Subsequently, using a 1D toy potential model, we solve the corresponding time independent Schrödinger equation for the stationary scattering states and calculate the transmission coefficient. We also solve the associated bound state boundary value problem.

In **Chapter 2** we introduce and explore the theory of NHQM. First, we

mathematically describe the concept of Gamow-Siegert states (bound states, anti-bound states, resonances, anti-resonances), then discuss the different methods of approaching resonances and calculating their associated energies and wavefunctions. We illustrate these methods again on the same 1D toy potential model as in Chapter 1. Namely, we calculate the transmission probability and compare our results to the ones obtained in Chapter 1. Lastly, we briefly discuss the mathematical and physical properties of the anti-bound states.

In **Chapter 3** we focus on the problem of interaction of an atomic system with laser. We overview the basic underlying theoretical notions, most importantly, the gauge transformations, and the description of laser induced atomic resonances by means of the nonhermitian Floquet theory. Finally, as the ultimate "holy grail" of this thesis, we discuss the possible creation of a nonhermitian degeneracy known as an exceptional point (EP). We present an illustrative numerical calculation of an EP (for the same toy model as used in Chapters 1-2), and highlight some important, unusual, counter-intuitive properties of these EPs.

Chapter 1

Hermitian Scattering Theory

1.1 Introduction

This chapter will provide a brief outline of the quantum mechanical scattering theory embedded in the framework of conventional (hermitian) quantum mechanics. We will encounter along the way the phenomenon of scattering resonances, which will motivate us to switch into the nonhermitian quantum mechanical formalism in later chapters. The hermitian and nonhermitian approaches to quantum mechanics are equivalent and yield the same results for all physically observable quantities.

For the sake of maximum simplicity, all our theoretical explorations will concern one-dimensional single particle quantum systems. However, the presented formulations are generalizable rather straightforwardly to more complex systems of two or more quantum particles in three dimensions.

Let us consider a single non-relativistic quantum particle moving in one dimension in an external potential. The Hamiltonian of such a particle with mass m in potential field $V(x)$ is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\partial_{xx} + V(x) \quad ; \quad x \in (-\infty, +\infty) \quad . \tag{1.1}$$

The state vector $|\psi_t\rangle$, describing the quantum state of the particle at time t, evolves according to the Schrödinger equation

$$i\hbar\partial_t |\psi_t\rangle = \hat{H} |\psi_t\rangle \quad . \tag{1.2}$$

In what follows, we shall consider only short ranged potentials. Such that $V(x)$ falls off to zero quickly enough, i.e.

$$\lim_{x\to\pm\infty} x^3 V(x) = 0 \quad . \tag{1.3}$$

1.2 Time Dependent Scattering Theory

The Hilbert space of eigenstates of the Hamiltonian (1.1), $\mathcal{H}$, is divided into a discrete set of bound states $\mathcal{H}_B$ and a continuum of unbound states $\mathcal{H}_C$, i.e.

$$\mathcal{H} = \mathcal{H}_B \oplus \mathcal{H}_C \quad . \tag{1.4}$$

The time evolution operators for a free particle and a particle in a potential field $V(x)$, respectively, are

$$\hat{U}_0(t) = e^{-\frac{i}{\hbar}\hat{H}_0 t} \quad ; \tag{1.5}$$

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H} t} \quad ; \tag{1.6}$$

where

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\partial_{xx} \tag{1.7}$$

is the Hamiltonian of a free particle with mass m.

We will assume the satisfaction of the

Asymptotic Condition for Scattering [41]. *If the potential $V(x)$ satisfies the condition (1.3), then for $t \to \pm\infty$, the vector $|\psi_t\rangle$ evolves as a state vector describing a free particle, i.e. for every $|\psi_t\rangle \in \mathcal{H}_C$ there exist an incoming state $|\psi_{in}\rangle \in \mathcal{H}_C$ and an outgoing state $|\psi_{out}\rangle \in \mathcal{H}_C$ such that*

$$|\psi_t\rangle \Big|_{t\to-\infty} = \hat{U}_0(t)\,|\psi_{in}\rangle \quad ; \tag{1.8}$$

$$|\psi_t\rangle \Big|_{t\to+\infty} = \hat{U}(t)\,|\psi_{out}\rangle \quad . \tag{1.9}$$

1.2.1 Scattering Operator

We are interested in the overall output for scattering rather then the details of quantum dynamics at finite times. Our goal is, therefore, to calculate $|\psi_{\text{out}}\rangle$ using $|\psi_{\text{in}}\rangle$. We will do this by determining the scattering operator, $\boldsymbol{\hat{S} : \mathcal{H}_C \to \mathcal{H}_C}$, defined by

$$|\psi_{\text{out}}\rangle = \hat{S}\,|\psi_{\text{in}}\rangle \quad ; \tag{1.10}$$

which ***contains all physical information about scattering***.

Let us define $|\psi\rangle$ as the state vector of the particle at $t = 0$, i.e.

$$|\psi\rangle := |\psi_t\rangle \Big|_{t=0} \quad . \tag{1.11}$$

Using the properties of time evolution operators, $|\psi_t\rangle$ can be expressed as

$$|\psi_t\rangle = \hat{U}(t)\,|\psi\rangle \quad . \tag{1.12}$$

Let $T \to +\infty$. Then applying the asymptotic condition to (1.12) gives us

$$\begin{aligned} \hat{U}_0(-T)\,|\psi_{\text{in}}\rangle &= \hat{U}(-T)\,|\psi\rangle \quad ; \\ |\psi_{\text{in}}\rangle &= \hat{U}_0^\dagger(-T)\hat{U}(-T)\,|\psi\rangle \quad ; \end{aligned} \tag{1.13}$$

$$\begin{aligned} \hat{U}_0(+T)\,|\psi_{\text{out}}\rangle &= \hat{U}(+T)\,|\psi\rangle \quad ; \\ |\psi_{\text{out}}\rangle &= \hat{U}_0^\dagger(+T)\hat{U}(+T)\,|\psi\rangle \quad . \end{aligned} \tag{1.14}$$

Therefore,

$$|\psi_{\text{out}}\rangle = \hat{U}_0^\dagger(+T)\hat{U}(+T)\hat{U}^\dagger(-T)\hat{U}_0(-T)\,|\psi_{\text{in}}\rangle \quad . \tag{1.15}$$

Comparison of this result to the definition of $\hat{S}$, (1.10), shows us that

$$\boxed{\boldsymbol{\hat{S} = \hat{U}_0^\dagger(+T)\hat{U}(+T)\hat{U}^\dagger(-T)\hat{U}_0(-T)}} \quad . \tag{1.16}$$

Since $\hat{U}$ and $\hat{U}_0$ are unitary operators, $\hat{S}$ is unitary as well.

1.3 Time Independent Scattering Theory

The operator $\hat{S}$ is time independent, this motivates us to try to express it in a time independent way. It is the time independent formalism which gives deep physical insights into the quantum mechanical theory of scattering phenomena.

1.3.1 Free Particle

Let $|\phi_{E\eta}\rangle$ be eigenvectors of the free particle Hamiltonian $\hat{H}_0$, defined in (1.7), i.e.

$$\hat{H}_0 |\phi_{E\eta}\rangle = E |\phi_{E\eta}\rangle \tag{1.17}$$

$$-\frac{\hbar^2}{2m}\partial_{xx} |\phi_{E\eta}\rangle = E |\phi_{E\eta}\rangle \quad . \tag{1.18}$$

The solution to this differential equation is the plane wave

$$|\phi_{E\eta}\rangle = e^{iKx} \quad ; \tag{1.19}$$

where $K \in \mathbb{C}$. By substituting (1.19) back into (1.18) we get

$$-\frac{\hbar^2}{2m}\partial_{xx} e^{iKx} = E e^{iKx} \quad ; \tag{1.20}$$

$$\frac{\hbar^2 K^2}{2m} = E \quad . \tag{1.21}$$

Let $\eta := \operatorname{sgn}(K)$, then the wavenumber K can be written explicitly as

$$K = \frac{\eta}{\hbar}\sqrt{2mE} \quad . \tag{1.22}$$

Substitution of (1.21) into (1.20) results in the following equation:

$$-\frac{\hbar^2}{2m}\partial_{xx} e^{iKx} = \frac{\hbar K^2}{2m} e^{iKx} \tag{1.23}$$

$$\hat{p} e^{iKx} = \hbar K e^{iKx} \quad . \tag{1.24}$$

The plane wave (1.19) is, therefore, an eigenfunction of the momentum operator $\hat{p}$ and

$$p = \hbar K \quad . \tag{1.25}$$

We thus know the exact value of momentum p, which means that according to the Heisenberg uncertainty principle, the uncertainty of position x of a free particle is infinite.

Vectors $|\phi_{E\eta}\rangle$ make up an orthogonal basis of the Hilbert space $\mathcal{H}$. For the sake of simplification of later calculations, we require $|\phi_{E\eta}\rangle$ to be orthonormal; therefore,

$$\langle \phi_{E\eta} | \phi_{E'\eta'} \rangle = \delta(E - E')\delta_{\eta\eta'} \quad ; \tag{1.26}$$

$$\delta(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\xi\lambda}\,\mathrm{d}\xi \tag{1.27}$$

$$\Rightarrow \boldsymbol{\langle x | \phi_{e\eta} \rangle = \sqrt{\frac{m}{2\pi\hbar^2 |K|}}\, e^{\eta \frac{i}{\hbar}\sqrt{2mE}x}} \quad . \tag{1.28}$$

These vectors are not square-integrable and thus do not belong into the Hilbert space $\mathcal{H}$. They are improper vectors belonging into the rigged Hilbert space [3]. It can easily be shown that they also posses the closure property

$$\int_0^\infty \mathrm{d}E \sum_\eta |\phi_{E\eta}\rangle \langle \phi_{E\eta}| = \hat{I} \quad ; \tag{1.29}$$

where $\hat{I} : \mathcal{H} \to \mathcal{H}$ is an identity operator.

Since vectors $|\phi_{E\eta}\rangle$ make up a basis of $\mathcal{H} \supseteq \mathcal{H}_C$, there exist complex coefficients $C_{E\eta}$, $D_{E\eta}$ such that

$$|\phi_{\mathrm{in}}\rangle = \int_0^\infty \mathrm{d}E \sum_\eta C_{E\eta} |\phi_{E\eta}\rangle \quad ; \tag{1.30}$$

$$|\phi_{\mathrm{out}}\rangle = \int_0^\infty \mathrm{d}E \sum_\eta D_{E\eta} |\phi_{E\eta}\rangle \quad . \tag{1.31}$$

Due to orthonormality of this basis, these coefficients satisfy the following relations (Fourier coefficients):

$$C_{E\eta} = \langle \phi_{E\eta} | \phi_{\mathrm{in}} \rangle \quad ; \quad D_{E\eta} = \langle \phi_{E\eta} | \phi_{\mathrm{out}} \rangle \quad . \tag{1.32}$$

1.3.2 Lippmann-Schwinger Equation

It can be show that the following relations are also satisfied [38]:

$$|\psi\rangle = \int_0^\infty \mathrm{d}E \sum_\eta C_{E\eta} \left|\psi^+_{E\eta}\right\rangle \tag{1.33}$$

$$= \int_0^\infty \mathrm{d}E \sum_\eta D_{E\eta} \left|\psi^-_{E\eta}\right\rangle \quad ; \tag{1.34}$$

where $|\psi\rangle$ is the state of the system at $t = 0$, defined in (1.11), and vectors $\left|\psi^\pm_{E\eta}\right\rangle$ are be defined by the

Lippmann–Schwinger equation (LSE) [26]. *Let $\epsilon \to 0^+$, then*

$$\boxed{\left|\boldsymbol{\psi^\pm_{E\eta}}\right\rangle = |\boldsymbol{\phi_{E\eta}}\rangle + \frac{\mathbf{1}}{\boldsymbol{E - \hat{H} \pm i\epsilon}} \boldsymbol{\hat{V}} |\boldsymbol{\phi_{E\eta}}\rangle} \quad ; \tag{1.35}$$

where $\frac{1}{E-\hat{H}_0+i\epsilon}$ resp. $\frac{1}{E-\hat{H}_0-i\epsilon}$ is the retarded resp. advanced Green operator.

Theorem 1. *Let $\left|\psi^\pm_{E\eta}\right\rangle$ satisfy the Lippmann-Schwinger Equation (1.35), then $\left|\psi^\pm_{E\eta}\right\rangle$ also satisfies the Schrödinger equation*

$$\hat{H} \left|\psi^\pm_{E\eta}\right\rangle = E \left|\psi^\pm_{E\eta}\right\rangle \quad . \tag{1.36}$$

Proof. See Appendix A. □

Vectors $\left|\psi^{\pm}_{E\eta}\right\rangle$ are orthonormal, i.e.

$$\left\langle\psi^{\pm}_{E\eta}\middle|\psi^{\pm}_{E'\eta'}\right\rangle = \delta(E-E')\delta_{\eta\eta'} \quad . \tag{1.37}$$

And they posses the closure property

$$\int_0^\infty \mathrm{d}E \sum_\eta \left|\psi^{\pm}_{E\eta}\right\rangle \left\langle\psi^{\pm}_{E\eta}\right| = \hat{P} \quad ; \tag{1.38}$$

where $\hat{P} : \mathcal{H} \to \mathcal{H}_C$ is a projection operator into $\mathcal{H}_C$.

Using the relation (1.33) and the orthonormality of $|\phi_{E\eta}\rangle$, we get

$$\begin{aligned} D_{E'\eta'} = \left\langle\psi^{-}_{E'\eta'}\middle|\psi\right\rangle &= \int_0^\infty \mathrm{d}E \sum_\eta C_{E\eta} \left\langle\psi^{-}_{E'\eta'}\middle|\psi^{+}_{E\eta}\right\rangle = \\ &= \int_0^\infty \mathrm{d}E \sum_\eta \left\langle\psi^{-}_{E'\eta'}\middle|\psi^{+}_{E\eta}\right\rangle \left\langle\phi_{E\eta}|\phi_{\mathrm{in}}\right\rangle \quad . \end{aligned}$$

Substitution of this result into (1.31) then gives us

$$\begin{aligned} |\phi_{\mathrm{out}}\rangle &= \int_0^\infty \mathrm{d}E' \sum_{\eta'} D_{E'\eta'} \left|\phi_{E'\eta'}\right\rangle = \\ &= \int_0^\infty \mathrm{d}E' \sum_{\eta'} \int_0^\infty \mathrm{d}E \sum_\eta \left|\phi_{E'\eta'}\right\rangle \left\langle\psi^{-}_{E'\eta'}\middle|\psi^{+}_{E\eta}\right\rangle \left\langle\phi_{E\eta}|\phi_{\mathrm{in}}\right\rangle \quad . \end{aligned} \tag{1.39}$$

We again compare this equation to (1.10), seeing that

$$\boxed{\hat{\boldsymbol{S}} = \int_0^\infty \mathrm{d}\boldsymbol{E'} \sum_{\boldsymbol{\eta'}} \int_0^\infty \mathrm{d}\boldsymbol{E} \sum_{\boldsymbol{\eta}} \left|\boldsymbol{\phi_{E'\eta'}}\right\rangle \left\langle\boldsymbol{\psi^{-}_{E'\eta'}}\middle|\boldsymbol{\psi^{+}_{E\eta}}\right\rangle \left\langle\boldsymbol{\phi_{E\eta}}\right|} \quad . \tag{1.40}$$

This is the sought-after time-independent formula for $\hat{S}$, which reveals that ***all the information about scattering is encoded inside the LSE wavefunctions*** $\left|\boldsymbol{\psi^{\pm}_{E\eta}}\right\rangle$.

1.3.3 Reflection and Transmission

In what follows, we shall consider only the case where $\eta = +1$, and therefore $K > 0$ (the formulation for $\eta = -1$ would by analogical). It can be shown that functions $\psi^{+}_{E(+1)}(x)$ can be determined by solving the following differential equation [38]:

$$\left(-\frac{\hbar}{2m}\partial_{xx} + V(x)\right) \tilde{\psi}^{+}_{E(+1)}(x) = E\tilde{\psi}^{+}_{E(+1)}(x) \tag{1.41}$$

with the boundary conditions

$$\tilde{\psi}^{+}_{E(+1)}\left(x \to -\infty\right) = e^{iKx} + R(E)e^{-iKx} \quad ; \tag{1.42}$$

$$\tilde{\psi}^{+}_{E(+1)}\left(x \to +\infty\right) = T(E)e^{iKx} \quad ; \tag{1.43}$$

where $R(E)$ resp. $T(E)$ is the ***reflection*** resp. ***transmission coefficient***, the importance of which will be clarified later, and

$$\psi^{+}_{E(+1)} = \sqrt{\frac{m}{2\pi\hbar^2|K|}}\tilde{\psi}^{+}_{E(+1)}(x) \quad . \tag{1.44}$$

The wavefunction e^{iKx} describes the incoming free particle, $R(E)e^{-iKx}$ the reflected wave moving in the opposite direction and $T(E)e^{iKx}$ the transmitted wave that has passed through the potential barrier.

Boundary conditions (1.42)-(1.43) tell us that for $x \to -\infty$, $\psi^{+}_{E\eta}(x)$ is obtained as a superposition of the incoming and the reflected wave. And that for $x \to +\infty$, $\psi^{+}_{E\eta}(x)$ is equal to the transmitted wave. The reflection resp. transmission coefficient is defined as the ratio of the amplitude of the reflected resp. transmitted wave to the amplitude of the incoming wave. ***These coefficients ultimately include all the information about scattering*** and are thus equivalent to $\hat{S}$. Namely $|\phi_{\text{out}}\rangle$ can be obtained from $|\phi_{\text{in}}\rangle$ using the following equation [38]:

$$|\phi_{\text{out}}\rangle = \left|\phi^{T}_{\text{out}}\right\rangle + \left|\phi^{R}_{\text{out}}\right\rangle \quad ; \tag{1.45}$$

where

$$\left|\phi^{R}_{\text{out}}\right\rangle = \int_0^\infty \mathrm{d}E \, \left|\phi_{E(-1)}\right\rangle R^{+}_{E(+1)} \left\langle\phi_{E(+1)}\middle|\phi_{\text{in}}\right\rangle \quad ; \tag{1.46}$$

$$\left|\phi^{T}_{\text{out}}\right\rangle = \int_0^\infty \mathrm{d}E \, \left|\phi_{E(+1)}\right\rangle T^{+}_{E(+1)} \left\langle\phi_{E(+1)}\middle|\phi_{\text{in}}\right\rangle \quad . \tag{1.47}$$

Since the reflection and transmission coefficients are complex numbers $\forall E \in \mathbb{R}^+$, they can be expressed in the following forms:

$$R(E) = |R(E)|e^{i\arg(R(E))} \quad ; \tag{1.48}$$

$$T(E) = |T(E)|e^{i\arg(T(E))} \quad . \tag{1.49}$$

The values of $|R(E)|^2$ resp. $|T(E)|^2$ corresponds to the probability of reflection. resp. transmission and satisfy the ***probability conservation***[1]

$$|T(E)|^2 + |R(E)|^2 = 1 \quad . \tag{1.50}$$

The phase $\arg(T(E))$ factors in determining the so-called ***Eisenbud-Wigner-Smith time delay***, which tells us how long a particle stays in the interaction region and can be calculated as [10]

$$\tau = \hbar\partial_E \arg(T(E)) \quad . \tag{1.51}$$

Let us now find an explicit formula for the transmission coefficient $T(E)$. The expression (1.40) tells us that the matrix elements of $\hat{S}$ can be calculated as

$$S_{(E\eta)(E'\eta')} = \langle\phi_{E\eta}|\,\hat{S}\,|\phi_{E'\eta'}\rangle = \left\langle\psi^{-}_{E\eta}\middle|\psi^{+}_{E'\eta'}\right\rangle \quad . \tag{1.52}$$

It can be shown that the following formula for $S_{(E\eta)(E'\eta')}$ applies [38]:

$$S_{(E\eta)(E'\eta')} = \delta(E-E')\delta_{\eta\eta'} - 2i\pi\delta(E-E')T_{(E\eta)(E'\eta')} \quad ; \tag{1.53}$$

[1] Proof in appendix B.

where by definition

$$T_{(E\eta)(E'\eta')} \coloneqq \langle \phi_{E\eta} | \hat{V} | \psi_{E\eta^+} \rangle = \langle \phi_{E\eta} | \hat{V} + \hat{V} \frac{1}{E - \hat{H} + i0_+} \hat{V} | \phi_{E\eta'} \rangle \quad . \tag{1.54}$$

These entities are the so-called on-shell T-matrix elements. They are the matrix elements of the transmission operator

$$\hat{T}(E) \coloneqq \hat{V} + \hat{V} \frac{1}{E - \hat{H} + i\epsilon} \hat{V} \quad . \tag{1.55}$$

It can be shown that, using this operator, we can calculate the value of the transmission coefficient as [38]

$$\boxed{\boldsymbol{T(E) = 1 - 2\pi i \langle \phi_{E(+1)} | \hat{V} + \hat{V} \frac{1}{E - \hat{H} + i\epsilon} \hat{V} | \phi_{E(+1)} \rangle}} \quad . \tag{1.56}$$

This relation equivalent to the Lippmann-Schwinger equation (1.35).

1.4 Numerical Solution of the Time Independent Schrödinger Equation for the Stationary Scattering States

We are unable to solve the boundary value problem (1.41)-(1.43) analytically for general $V(x)$. We can, however, use numeric methods to get an approximate solution to any degree of accuracy. We will do this by approximating the differential equation (1.41) by a difference equation.

1.4.1 Difference Approximation

First, we divide the x axis into an equidistant grid, with the distance between grid points of Δx, and define

$$\forall n \in \mathbb{Z} \quad ; \quad x_n \coloneqq n\Delta x \quad ; \tag{1.57}$$

$$\tilde{\psi}_n \coloneqq \tilde{\psi}^+_{E(+1)}(x_n) \quad . \tag{1.58}$$

Using the Taylor expansion of $\tilde{\psi}^+_{E(+1)}(x \pm h)$ for $h > 0$ we get

$$\tilde{\psi}^+_{E(+1)}(x+h) = \tilde{\psi}^+_{E(+1)}(x) + (\tilde{\psi}^+_{E(+1)})'(x)h + \frac{1}{2}(\tilde{\psi}^+_{E(+1)})''(x)h^2 + O(h^3) \quad ; \tag{1.59}$$

$$\tilde{\psi}^+_{E(+1)}(x-h) = \tilde{\psi}^+_{E(+1)}(x) - (\tilde{\psi}^+_{E(+1)})'(x)h + \frac{1}{2}(\tilde{\psi}^+_{E(+1)})''(x)h^2 + O(h^3) \quad . \tag{1.60}$$

Adding up these two equations gives us

$$\tilde{\psi}^+_{E(+1)}(x+h) + \tilde{\psi}^+_{E(+1)}(x-h) = 2\tilde{\psi}^+_{E(+1)}(x) + (\psi^+_{E(+1)})''(x)h^2 + O(h^4) \quad ; \tag{1.61}$$

and thus

$$(\tilde{\psi}^{+}_{E(+1)})''(x) = \frac{\tilde{\psi}^{+}_{E(+1)}(x+h) - 2\tilde{\psi}^{+}_{E(+1)}(x) + \tilde{\psi}(x-h)}{h^2} + O(h^4) \quad . \tag{1.62}$$

For $h = \Delta x$; therefore,

$$\tilde{\psi}''_n \approx \frac{\tilde{\psi}_{n+1} - 2\tilde{\psi}_n + \tilde{\psi}_{n-1}}{(\Delta x)^2} \quad ; \tag{1.63}$$

and

$$\boxed{-\frac{\boldsymbol{\hbar^2}}{\boldsymbol{2m}}\left(\frac{\tilde{\boldsymbol{\psi}}_{\boldsymbol{n+1}} - \boldsymbol{2\tilde{\psi}_n} + \tilde{\boldsymbol{\psi}}_{\boldsymbol{n-1}}}{\boldsymbol{(\Delta x)^2}}\right) + \boldsymbol{V(x_n)\tilde{\psi}_n \approx E\tilde{\psi}_n}} \quad . \tag{1.64}$$

Using this relation, we can propagate $\tilde{\psi}_n$ left and right when knowing two adjacent values of $\tilde{\psi}_n$. This is equivalent to knowing the values of $\tilde{\psi}_n$ and $\tilde{\psi}'_n$ in a single point (initial conditions).

The boundary conditions (1.42)-(1.43) can be rewritten with a convenient wavefunction renormalization as

$$\tilde{\psi}^{+}_{E(+1)}\,(x \to -\infty) = A(E)e^{iKx} + B(E)e^{-iKx} \quad ; \tag{1.65}$$

$$\tilde{\psi}^{+}_{E(+1)}\,(x \to +\infty) = e^{iKx} \quad ; \tag{1.66}$$

where

$$T(E) = \frac{1}{A(E)} \quad ; \quad R(E) = \frac{B(E)}{A(E)} \quad . \tag{1.67}$$

The conditions (1.65)-(1.66) allow us to approximate the value of $\tilde{\psi}(x)$ for large values of $|x|$. Let

$$x_1 = -\frac{L}{2} \quad ; \quad \Delta x = \frac{L}{N} \quad ; \quad L \in \mathbb{R}^+ \quad ; \quad N \in \mathbb{N} \tag{1.68}$$

(therefore, $x_N = \frac{L}{2}$), where L is large enough such that the values of $\tilde{\psi}^{+}_{E(+1)}(x)$ near the ends of the interval $(-\frac{L}{2}, \frac{L}{2})$ can be approximated using these boundary conditions. Values of $\tilde{\psi}_{N-1}$, $\tilde{\psi}_N$ can then be calculated as follows:

$$\tilde{\psi}_N = \tilde{\psi}^{+}_{E(+1)}(x_N) \approx e^{iKx_N} \quad ; \tag{1.69}$$

$$\tilde{\psi}_{N-1} = \tilde{\psi}^{+}_{E(+1)}(x_{N-1}) \approx e^{iKx_{N-1}} \quad . \tag{1.70}$$

We can now propagate $\tilde{\psi}_n$ left from these two points using (1.64). This allows us to compute $\tilde{\psi}_n, \forall n \in \{1, 2, \ldots N-1, N\}$. Thanks to the condition (1.65), the points $\tilde{\psi}_1$, $\tilde{\psi}_2$ satisfy the following relations:

$$\tilde{\psi}_1 = \tilde{\psi}^{+}_{E(+1)}(x_1) \approx A(E)e^{iKx_1} + B(E)e^{-iKx_1} \quad ; \tag{1.71}$$

$$\tilde{\psi}_2 = \tilde{\psi}^{+}_{E(+1)}(x_2) \approx A(E)e^{iKx_2} + B(E)e^{-iKx_2} \quad . \tag{1.72}$$

From these equations we can calculate the values of $A(E)$ and $B(E)$ and subsequently, using (1.67), the values of $T(E)$ and $R(E)$ to any degree of accuracy [30].

1.4.2 Toy Potential Model

We will now demonstrate this method using the toy potential

$$V(x) = (0.5x^2 - 0.8)e^{-0.1x^2} \quad . \tag{1.73}$$

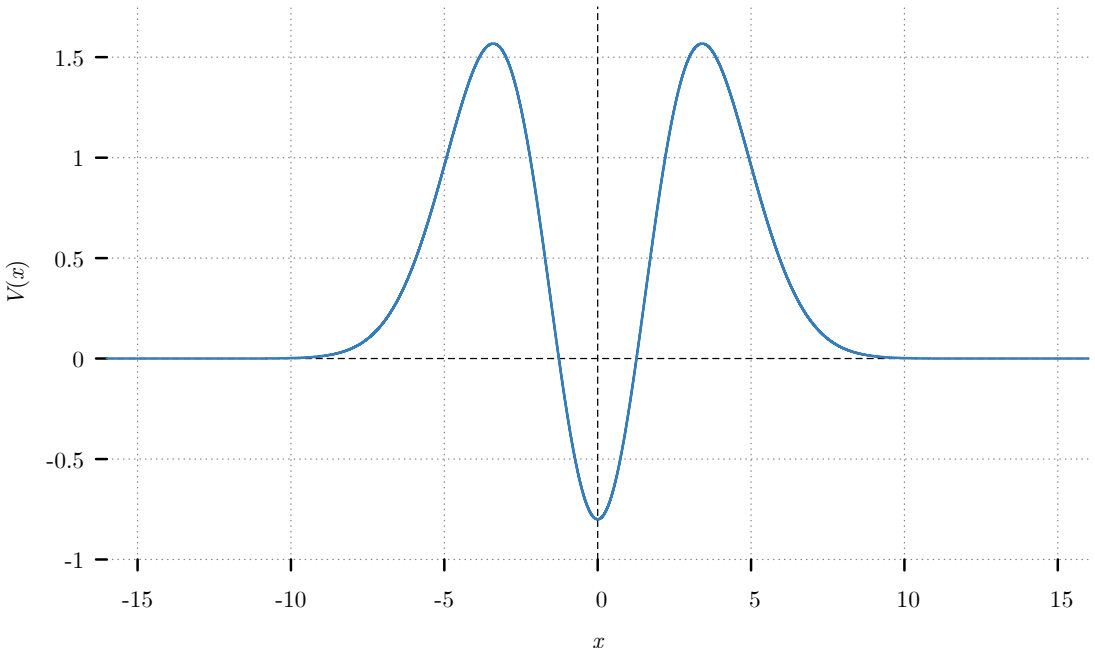

Figure 1.1: Two potential barriers are separated by potential well, suggesting that a quantum particle of positive energy can be temporarily trapped between the barriers.

using arbitrary (dimensionless) units and setting

$$\hbar = 1 \quad ; \quad m = 1 \tag{1.74}$$

and

$$N = 10^6 \quad ; \quad L = 50 \tag{1.75}$$

(therefore, $x_1 = -25$, $x_N = 25$).

Formula (1.50) will be used as a precision check. The closer the value of $|T(E)|^2 + |R(E)|^2$ is to 1 when using our calculated values of $T(E)$, $R(E)$, the better precision we have achieved.

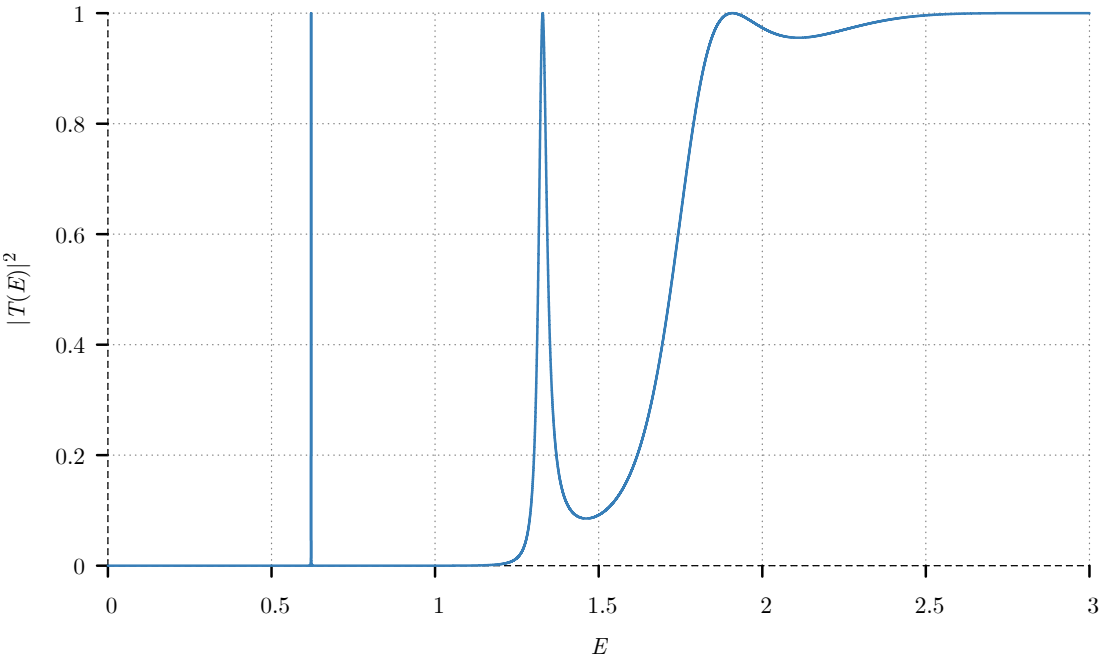

Figure 1.2: transmission probability $|T(E)|^2$. For certain energies peaks in the transmission probability occur. These energies correspond to phenomena known as ***resonances***, which will be discussed in detail in Chapter 2. There we will employ the methods of NHQM to clearly define them and to associate each resonance with only a single energy level, as opposed to the interval associated with each peak currently. As we can see, the second peak is much broader than the first one and the third one even more so. This suggests that there may be other resonances that are very broad and overlapping and as such cannot be clearly seen in this graph. This is an issue, which will also be solved in Chapter 2 using methods of NHQM.

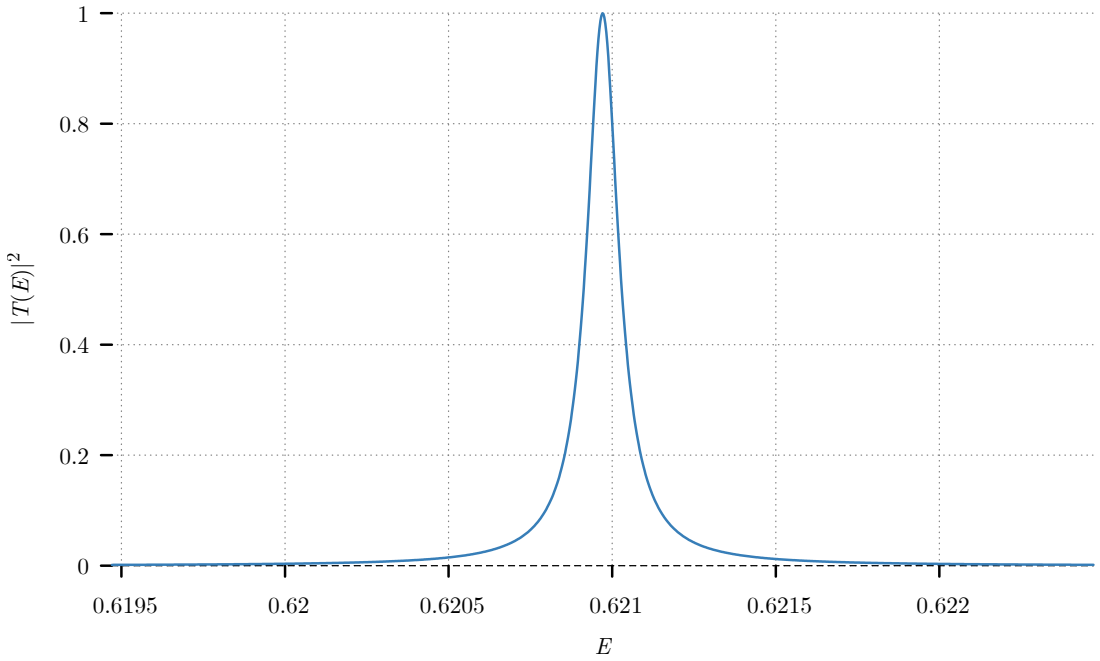

Figure 1.3: Zoom on the first peak corresponding to energy $E = 0.62097$. We see that the function reaches the maximum value of 1 at the point $E = 0.62097$ and then quickly dies down to zero.

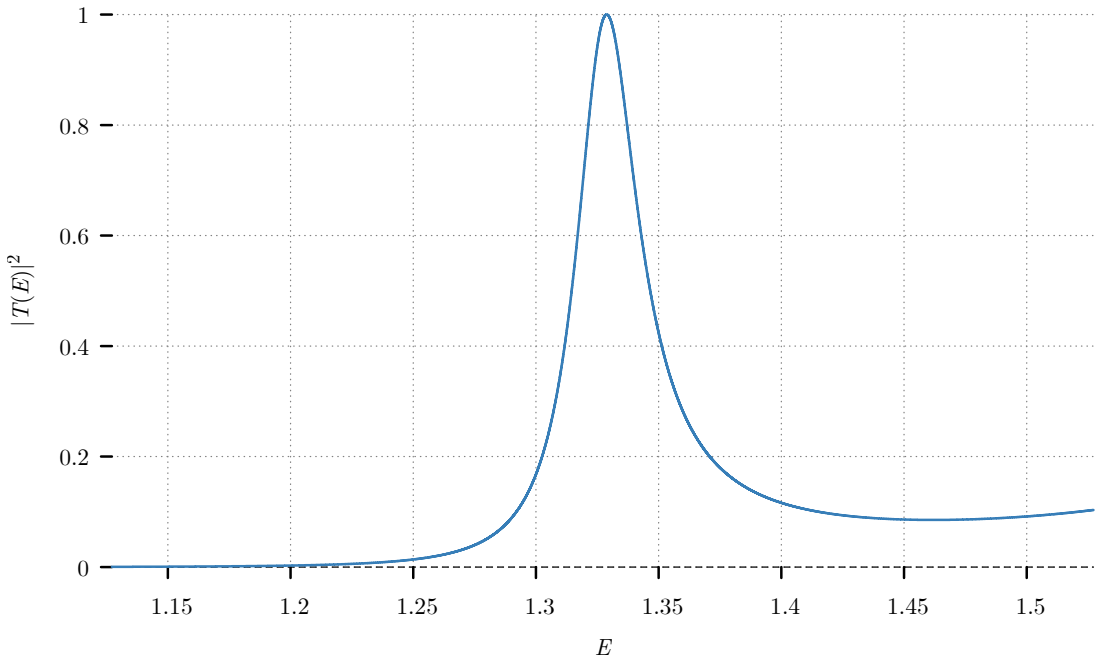

Figure 1.4: Zoom on the second peak corresponding to energy $E = 1.32720$.

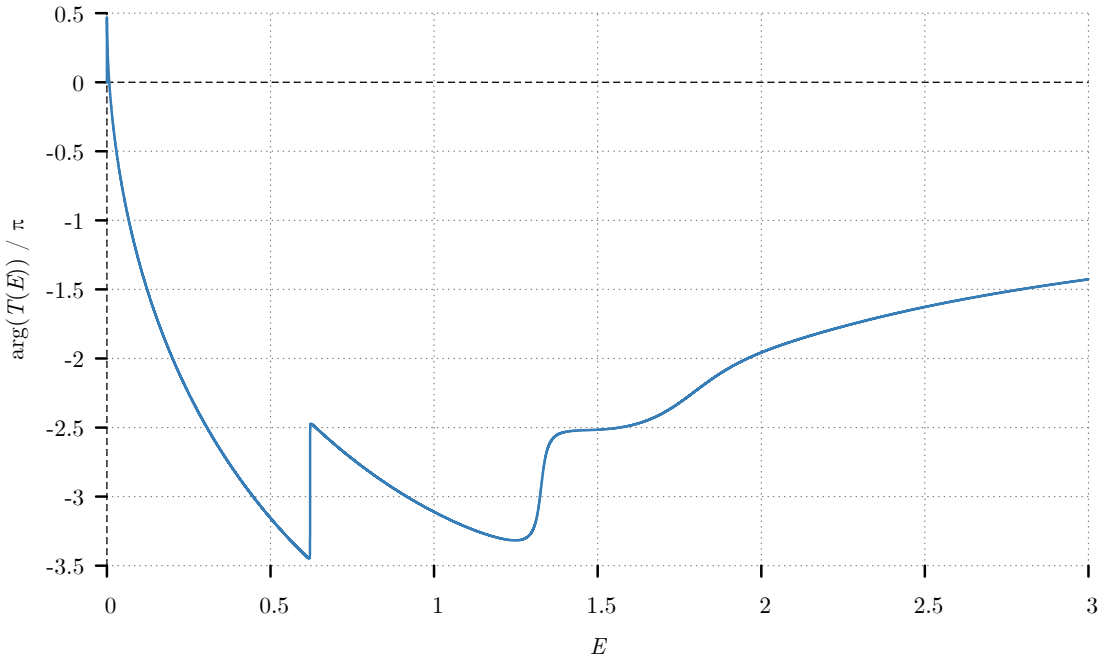

Figure 1.5: Phase of $T(E)$ divided by π. We observe abrupt jumps in the phase of $T(E)$ at the same energies as the previously discussed peaks in probability. This causes large Eisenbud-Wigner-Smith times for these energies, see (1.51).

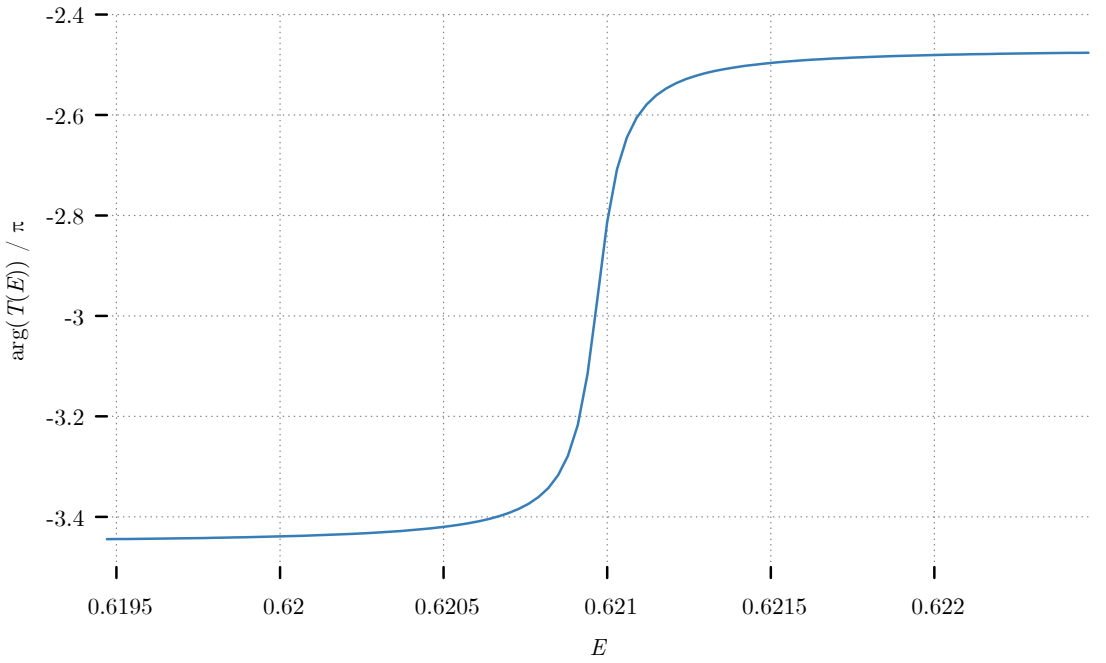

Figure 1.6: Zoom on the first jump corresponding to energy $E = 0.62097$. We see that the change in $\arg(T(E))$ is continuous and that the magnitude of the jump is roughly π.

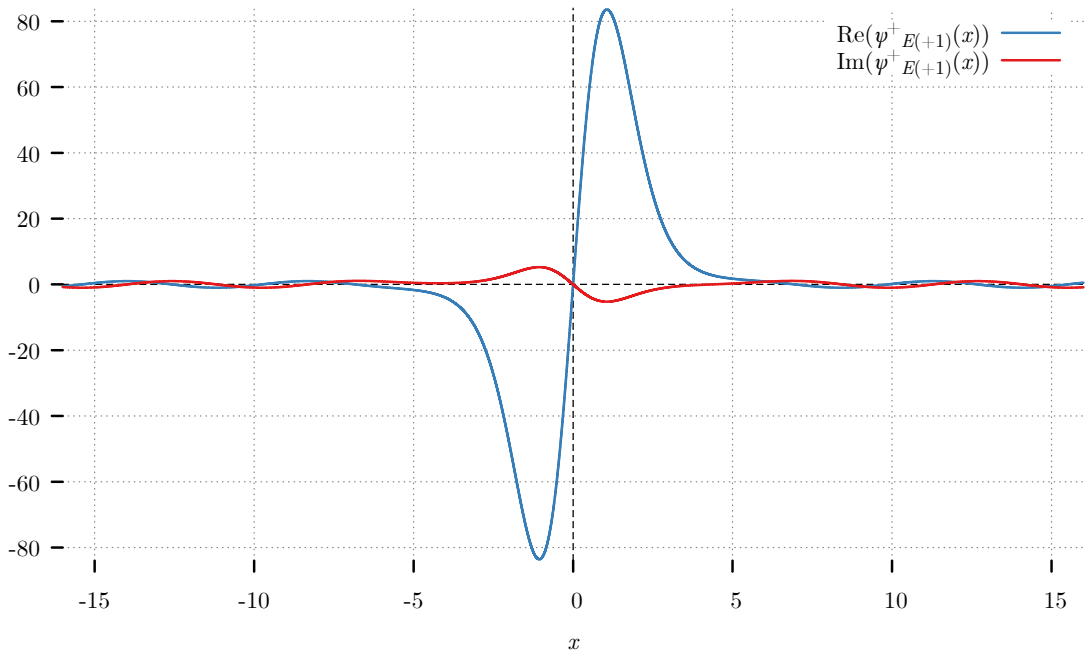

Figure 1.7: Real and imaginary parts of the eigenfunction of $\hat{H}$ corresponding to first resonance energy $E = 0.62097$. The wavefunction is highly localized similarly to a bound state, and its nodal structure closely resembles the nodal structure of the second bound state of the linear harmonic oscillator (LHO). This is quite an atypical behavior for an unbound eigenstate of $\hat{H}$.

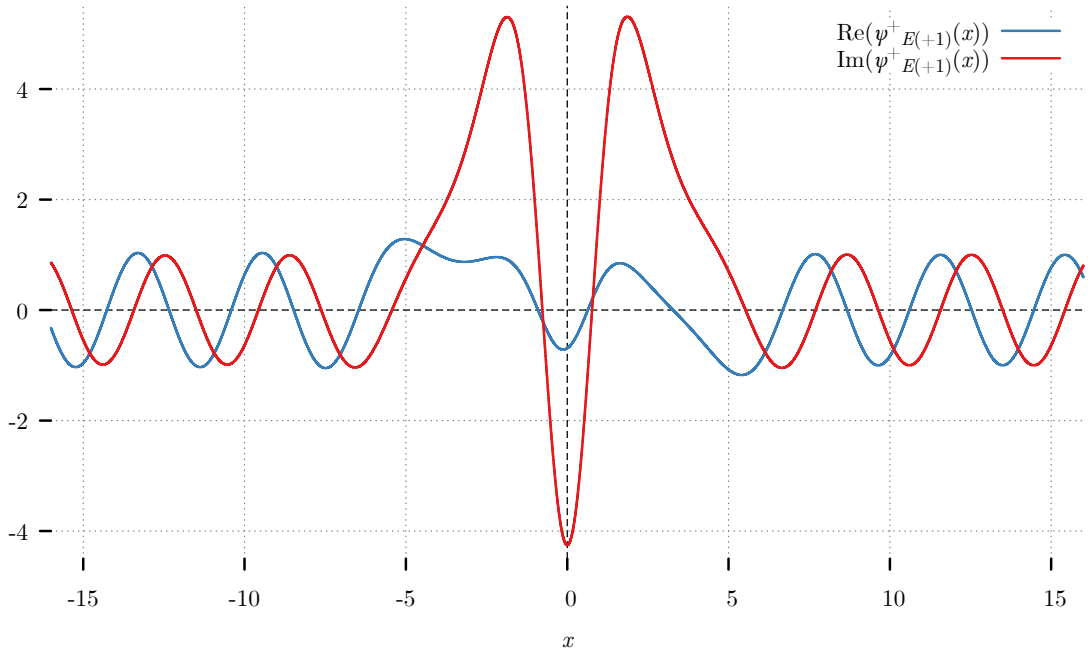

Figure 1.8: Real and imaginary parts of the eigenfunction of $\hat{H}$ corresponding to second resonance energy $E = 1.32720$. The wavefunction is again partially localized; however, to a lesser degree than in Figure 1.7. Its nodal structure resembles the nodal structure of the third bound state of the LHO. This is again not behavior we would expect from an unbound eigenstate of $\hat{H}$.

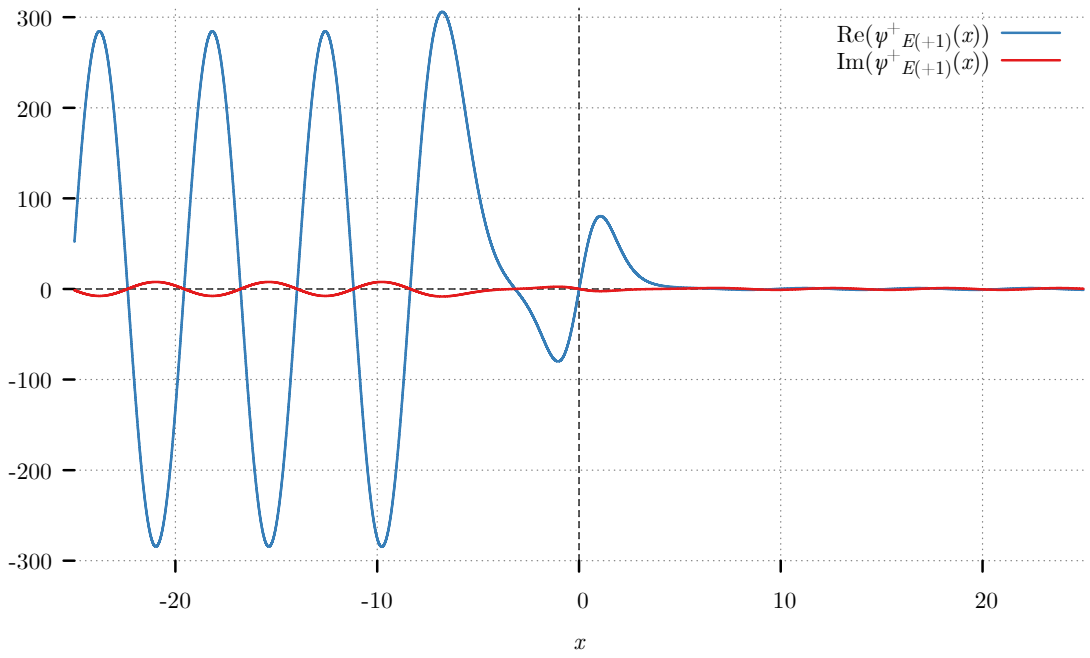

Figure 1.9: Real and imaginary parts of the eigenfunction of $\hat{H}$ corresponding to the energy $E = 0.63$, which is only slightly different from the energy used in Figure 1.7. As we can see, even a small departure from the resonance energy results in the eigenfunction no longer being localized with a nodal structure no longer resembling a bound state of the LHO.

These results point out a similarity between resonances and bound states. However, unlike with bounds states, standard quantum mechanics lacks the tools to efficiently describe resonances and is unable to associate them with a single energy level. These problems will be remedied by NHQM in Chapter 2.

1.5 Bound States

In this section, we will investigate the problem of solving the Schrödinger equation for bound states. This will prove a useful analogy for studying phenomena in NHQM such as resonances and exceptional points, see Chapters 2-3.

We are solving the equation

$$\left(-\frac{\hbar}{2m}\partial_{xx} + V(x)\right)\psi(x) = E\psi(x) \quad ; \tag{1.76}$$

with the ***bound state boundary conditions***

$$\psi\left(x \to \pm\infty\right) = 0 \quad . \tag{1.77}$$

Let $(b_j(x))_{j=1}^{\infty}$ be a discrete orthonormal basis of $\mathrm{L}^2(\mathbb{R})$. The function $\psi(x)$ can then be expanded as

$$\psi(x) = \sum_{j=1}^{\infty} c_j b_j(x) \quad ; \tag{1.78}$$

where

$$c_j = \langle b_j | \psi \rangle \quad . \tag{1.79}$$

After substituting (1.76) into (1.78) we get

$$\left(-\frac{\hbar^2}{2m} \partial_{xx} + V(x) \right) \sum_{j'} c_{j'} b_k(x) = E \sum_{j'} c_{j'} b_{j'}(x) \quad \Big| \int_{-\infty}^{+\infty} \mathrm{d}x \, b_j^*(x)$$

$$\sum_{j'} c_{j'} \langle b_j | - \frac{\hbar^2}{2m} \partial_{xx} | b_{j'} \rangle + \sum_{j} c_{j'} \langle b_j | V(x) | b_{j'} \rangle = E c_j \quad . \tag{1.80}$$

Using Hamiltonian matrix elements

$$H_{jj'} \coloneqq \langle b_j | - \frac{\hbar^2}{2m} \partial_{xx} | b_{j'} \rangle + \langle b_j | V(x) | b_{j'} \rangle = H_{j'j}^* \quad ; \tag{1.81}$$

we can then rewrite (1.80) as

$$\sum_{j'} H_{jj'} c_{j'} = E c_j \quad ;$$

$$\boxed{\underline{\underline{\boldsymbol{H}}} \, \vec{\boldsymbol{c}} = \boldsymbol{E} \vec{\boldsymbol{c}}} \quad ; \tag{1.82}$$

where $\underline{\underline{H}}$ is an infinite hermitian matrix and $\vec{c}$ an infinite arithmetical column vector. In numerical calculations they will be approximated by finite ones (basis set truncation). We have thus converted the operator eigenvalue problem (1.76)-(1.77) into a matrix eigenvalue problem of linear algebra. This approach is equivalent to using the quantum mechanical variation principle [15].

A crucial part of the calculation is an appropriate choice of the basis set. We will use the particle-in-the-box basis set

$$b_j(x) \coloneqq \sqrt{\frac{2}{L}} \sin\left(\frac{j\pi}{L} \left(x - \frac{L}{2} \right) \right) \quad ; \quad j \in \mathbb{N} \quad ; \tag{1.83}$$

for $L \in \mathbb{R}^+$ large enough for the potential $V(x)$ to be essentially zero $\forall x \in \mathbb{R} \setminus (-L, L)$, and for bound states to be independent of L. This basis is orthonormal, i.e.

$$\langle b_j | b_{j'} \rangle = \delta_{jj'} \quad ; \quad \forall j, j' \in \mathbb{N} \quad ; \tag{1.84}$$

and satisfies the closure property

$$\sum_{j} b_j(x) b_j^*(x') = \delta(x - x'), \quad \forall x, x' \in \left(-\frac{L}{2}, \frac{L}{2} \right) \quad . \tag{1.85}$$

1.5.1 Toy Potential Model

We will now find a numerical solution to algebraic eigenvalue problem (1.82) for toy potential (1.73) in arbitrary units, while setting (1.74).

The following relations will be used when calculating the elements of $\underline{\underline{H}}$:

$$\langle b_j | V(x) | b_{j'} \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) V(x) b_{j'}(x) = \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, (0.5x^2 - 0.8) e^{-0.1x^2} b_j(x) b_{j'}(x) \quad ; \tag{1.86}$$

$$\begin{aligned} \langle b_j | -\frac{\hbar^2}{2m}\partial_{xx} | b_{j'} \rangle &= \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) \left(-\frac{\hbar^2}{2m}\partial_{xx} \right) b_{j'}(x) = \\ &= \frac{\hbar^2}{2m} \frac{(j')^2 \pi^2}{L^2} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) b_{j'}(x) = \frac{\hbar^2}{2m} \frac{(j')^2 \pi^2}{L^2} \delta_{jj'} \quad . \end{aligned} \tag{1.87}$$

The basis set was truncated to include only the first $N \in \mathbb{N}$ functions. The calculations were done using values of N of 100, 200 and 400 and values of L of 50 and 100. The integration was done numerically with step size of $\mathrm{d}x = \frac{L}{10^6}$. The eigenvalue problem was then solved using the Eigen [16] package for C++.

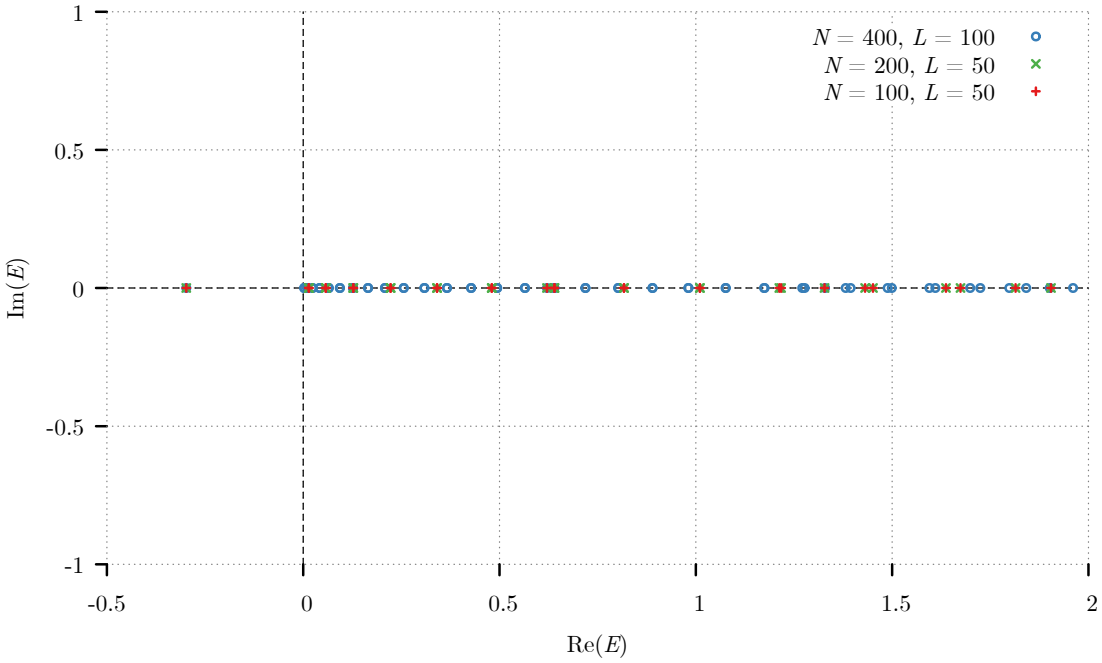

Figure 1.10: Resulting energy eigenvalues composed of a single bound state with energy $E_0 = -0.29796$ and a positive energy continuum. We see that the larger values of N and L we use, the more points are generated, as our approximations get better and the positive energy spectrum closer resembles continuum. Since the Hamiltonian (1.1), appearing in Equation (1.76), is hermitian, all the resulting eigenvalues are strictly real. They were plotted in the complex plane to better illustrate the relation to the complex eigenvalues we will see later in Chapter 2, where the algorithm will be generalized to the complex plane.

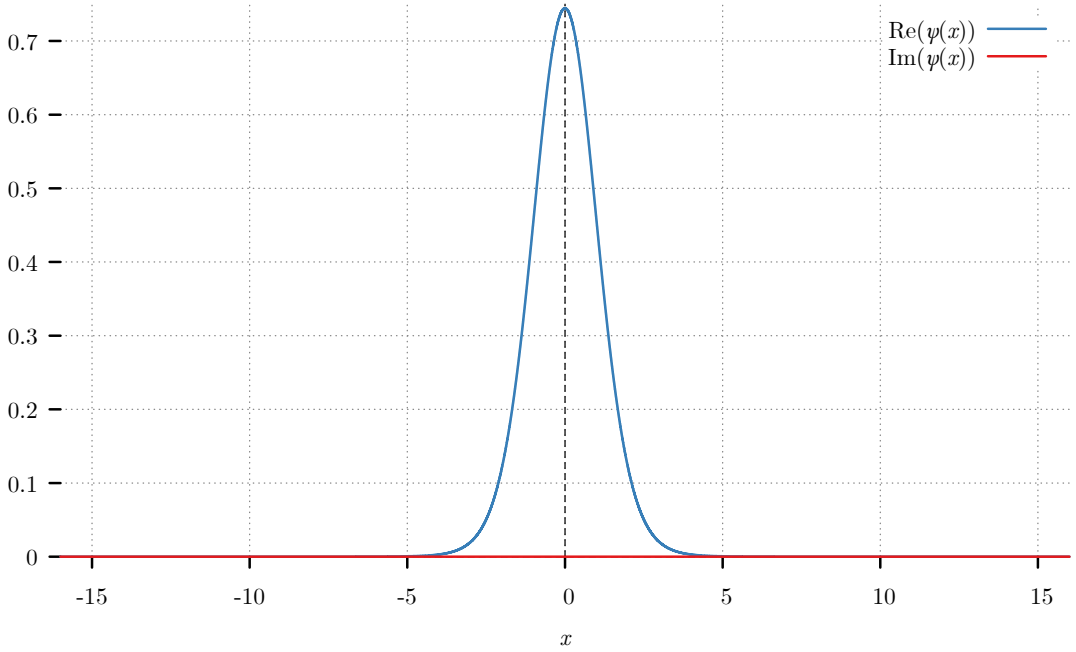

Figure 1.11: Real and imaginary parts of the first and only bound state with energy $E_0 = -0.29796$ for $N = 400$, $L = 50$. As we can see, it is completely localized in the interaction region $(-\frac{L}{2}, \frac{L}{2})$.

1.6 Summary

We have outlined the formalism of hermitian scattering theory, calculated the ***scattering operator*** $\hat{S}$ in a time independent way using LSE wavefunctions and described ***reflection*** and ***transmission*** using the reflection and transmission coefficients. We have subsequently, with the help of numerical models, solved the ***time independent Schrödinger equation for stationary scattering states*** and the ***bound state boundary value problem*** and calculated the values of the ***transmission coefficient*** for a toy potential model in one dimension. Results obtained for physically observable quantities, such as the transmission probability, will be used as a standard to check our results against in Chapter 2.

In our results we have noticed the phenomenon of ***scattering resonances*** and plotted the state vectors associated with them. Our inability to satisfactorily predict and describe these phenomena motivates us to switch to a nonhermitian approach.

Chapter 2

Nonhermitian Quantum Mechanics

2.1 Introduction and Motivation

For studying and sharply defining resonances, it would be convenient for us to be able to associate each resonance with a single eigenstate of $\hat{H}$ and a single energy level. This can be done by solving the following familiar eigenvalue problem

$$\left(-\frac{\hbar^2}{2m}\partial_{xx} + V(x)\right)\psi(x) = E\psi(x) \quad ; \tag{2.1}$$

but this time allowing $E \in \mathbb{C}$ and imposing a special kind of boundary conditions called the ***Siegert type boundary conditions***.

To better describe resonances and other related phenomena we will now generalize the notion of bound states from HQM into the so-called ***Gamow-Siegert states***.

2.1.1 Gamow-Siegert States

The Gamow-Siegert states, first conceived by G. Gamow and A. F. J. Siegert in 1939 [36], are defined as the solutions to Equation (2.1) with the Siegert type boundary conditions

$$\psi\left(x \to -\infty\right) = C_- e^{-iKx} = C_- e^{-iK_1 x} e^{K_2 x} \quad ; \tag{2.2}$$

$$\psi\left(x \to +\infty\right) = C_+ e^{iKx} = C_+ e^{iK_1 x} e^{-K_2 x} \quad ; \tag{2.3}$$

where

$$C_-, C_+ \in \mathbb{C} \tag{2.4}$$

and

$$K = \frac{1}{\hbar}\sqrt{2mE} =: K_1 + iK_2, \quad ; \quad K_1, K_2 \in \mathbb{R} \quad . \tag{2.5}$$

We see that each Siegert type boundary condition consists of only a ***single exponential***, as opposed to the more general superposition of two. It can be shown that the boundary conditions (2.2)-(2.3) result in energy being quantized [29]. One may also notice that with these boundary conditions

$$\psi(x \to \pm\infty) = \infty \iff K_2 < 0 \quad ; \tag{2.6}$$

where ∞ denotes the complex infinity. Therefore, not all Gamow-Siegert states are square-integrable and thus ***do not belong into the domain of HQM***.

2.1.2 Classification of Gamow-Siegert States

For future calculations it will be convenient to divide the Gamow-Siegert states into several categories depending on the value of K. The categories are as follows:

Bound States

Let us first consider the situation where K is strictly imaginary and its imaginary part positive, i.e.

$$K = i\kappa \quad ; \quad \kappa \in \mathbb{R}^+ \quad ; \tag{2.7}$$

and therefore

$$E = -\frac{\hbar^2\kappa^2}{2m} \in \mathbb{R}^- \quad . \tag{2.8}$$

The boundary conditions (2.2)-(2.3) then become

$$\psi\left(x \to \pm\infty\right) = e^{\mp\kappa x} = 0 \quad . \tag{2.9}$$

We notice that the expression (2.9) is identical to the bound state boundary conditions (1.77). The Gamow-Siegert states are, therefore, in this case, the already familiar bound states discussed in Chapter 1.

Anti-bound states

This situation occurs when K is strictly imaginary and its imaginary part is negative, i.e.

$$K = -i\kappa \quad ; \quad \kappa \in \mathbb{R}^+ \quad ; \tag{2.10}$$

therefore again

$$E = -\frac{\hbar^2\kappa^2}{2m} \in \mathbb{R}^- \tag{2.11}$$

and

$$\psi\left(x \to \pm\infty\right) = e^{\pm iKx} = e^{\pm\kappa x} = \infty \quad . \tag{2.12}$$

Anti-bound states thus explode as x approaches $\pm\infty$. Therefore, the are not square-integrable and as such do not represent a state of a quantum particle.

Resonances and Anti-Resonances

These situations occur when K is not strictly real or strictly imaginary, i.e.

$$K_1 \neq 0 \quad ; \quad K_2 \neq 0 \quad ; \tag{2.13}$$

and therefore

$$E = -\frac{\hbar^2}{2m}\left(K_1^2 - K_2^2\right) + i\frac{\hbar}{2m}2K_1K_2 \in \mathbb{C} \quad . \tag{2.14}$$

Let us now assume that $K_2 > 0$, then $\psi(x)$ would be a square-integrable eigenstate of $\hat{H}$, but since $\hat{H}$ is a hermitian operator, E would have to be a real number. This is contradictory to (2.14). Therefore,

$$K_2 < 0 \quad . \tag{2.15}$$

We call these states ***resonances*** when $K_1 > 0$, and therefore $\mathrm{Im}(E) < 0$ and ***anti-resonances*** when $K_1 < 0$ and therefore $\mathrm{Im}(E) > 0$. It will later be shown that resonances defined in this manner indeed correspond to the resonance phenomenon encountered in Chapter 1, plotted in Figure 1.2. We notice that both resonances and anti-resonances explode for $x \to \pm\infty$, and are consequently also not square-integrable.

We are able to switch between resonances and anti-resonances by applying complex conjugation to (2.1):

$$\left(-\frac{\hbar^2}{2m}\partial_{xx} + V(x)\right)\psi(x) = E\psi(x) \quad \Big|^* \quad ; \tag{2.16}$$

$$\left(-\frac{\hbar^2}{2m}\partial_{xx} + V(x)\right)\psi^*(x) = E^*\psi^*(x) \quad . \tag{2.17}$$

This gives us an equivalent eigenproblem with complex conjugated energy and boundary conditions

$$\psi^*\left(x \to \pm\infty\right) = e^{\mp iK_1 x} e^{\mp K_2 x} \quad . \tag{2.18}$$

As we can see, the only difference is that K_1 switched signs. Therefore, for $K_1 > 0$ we have obtained an anti-resonance ψ^* from the resonance ψ and vice versa for $K_1 < 0$.

$K \in \mathbb{R}\backslash\{0\}$

A situation where $K \in \mathbb{R}\backslash\{0\}$ is impossible, see appendix C.

$K = 0$

The last possible option is for K to be equal to zero. Therefore, $E = 0$ and

$$e^{iKx} = e^{-iKx} = 1 \quad . \tag{2.19}$$

This makes the Siegert type boundary conditions (2.2)-(2.3) ill-defined, and we thus discard this situations from our considerations.

2.1.3 Further Comments

Since resonances are not square-integrable, they are not normalizable in the usual sense. (We will later define the so-called C-normalization, in respect to which it will be possible to normalize them.) This greatly complicates working with them. There are two currently known ways of getting around this problem: the ***complex coordinate method*** also known as complex scaling (CS) and the ***method of Siegert pseudostates***. We will now describe both of them in detail, starting with the complex coordinate method.

2.2 Complex Coordinate Method

2.2.1 Introduction

The core of this method lies in modifying the resonance wave functions in such a way that they become square-integrable. This will be done by rotating the resonance states into the complex plane using ***analytic continuation*** [2].

2.2.2 Boundary Conditions

As previously stated, resonances satisfy the Siegert type boundary conditions (2.2)-(2.3) with

$$K = K_1 + iK_2 \quad ; \quad K_1 > 0 \quad ; \quad K_2 < 0 \quad ; \tag{2.20}$$

and therefore

$$\psi\left(x \to \pm\infty\right) = e^{\pm iK_1 x} e^{\mp K_2 x} = \infty \quad . \tag{2.21}$$

But in order for the function ψ to be square-integrable, it needs to decay for $x \to \pm\infty$. We will achieve this by substitution of a complex variable. Let us denote

$$\vartheta \coloneqq -\arg(K) \quad . \tag{2.22}$$

We can then write

$$K = |K|e^{-i\vartheta} \quad ; \quad e^{iK_1 x} e^{-K_2 x} = \exp\left(i|K|xe^{-i\vartheta}\right) \quad . \tag{2.23}$$

Next we substitute x with the complex variable

$$z \coloneqq xe^{i\theta} \in \mathbb{C} \quad ; \quad \theta \in \mathbb{R}^+ \quad ; \tag{2.24}$$

where θ is called the ***complex scaling angle***. This substitution transforms the wave function in the asymptotic regions into

$$e^{iKz} = \exp\left(i|K|xe^{-i(\theta-\vartheta)}\right) = e^{i|K|x\cos(\theta-\vartheta)} e^{-|K|x\sin(\theta-\vartheta)} \quad . \tag{2.25}$$

Therefore, since the exponential $e^{i|K|x\cos(\theta-\vartheta)}$ is oscillating, in order for e^{iKz} to decay for $x \to \pm\infty$, $\lim_{x\to\pm\infty} e^{-|K|x\sin(\theta-\vartheta)}$ must equal zero. This condition is satisfied when

$$\vartheta < \theta \quad . \tag{2.26}$$

Since for the bound state $K_1 = 0$ and thus

$$e^{iKz} = \exp\left(\mp K_2 xe^{i\theta}\right) = e^{\mp K_2 x\cos\theta} e^{\mp iK_2 x\sin\theta} \quad ; \tag{2.27}$$

then in order for e^{iKz} to decay for $x \to \pm\infty$, $\cos\theta$ needs to be negative, and therefore

$$\boldsymbol{\vartheta < \theta < \frac{\pi}{2}} \quad . \tag{2.28}$$

2.2.3 Analytic Continuation

We can now extend ψ into the complex plane using analytic continuation[1]. Let us define[2]

$$\varphi_\theta(x) \coloneqq \psi(z)e^{i\frac{\theta}{2}} = \psi(xe^{i\theta})e^{i\frac{\theta}{2}} \tag{2.29}$$

and substitute it into the boundary value problem (2.1), (2.3). This gives us

$$\begin{aligned} -\frac{\hbar^2}{2m}\partial_{zz}\psi(z) + V(x)\psi(z) &= E_\theta\psi(z) \\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(xe^{i\theta})^2}\varphi_\theta(x) + V(xe^{i\theta})\varphi_\theta(x) &= E_\theta\varphi_\theta(x) \\ \left(-\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta})\right)\varphi_\theta(x) &= E_\theta\varphi_\theta(x) \quad ; \end{aligned} \tag{2.30}$$

with boundary conditions

$$\varphi_\theta\left(x \to \pm\infty\right) = \exp\left(\pm iKxe^{i\theta}\right) = \exp\left(\pm i|K|e^{i(\theta-\vartheta)}\right) \quad . \tag{2.31}$$

We notice that the ***complex rotated Hamiltonian***

$$\boldsymbol{\hat{H}_\theta \coloneqq -\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta})} \quad ; \tag{2.32}$$

is ***not hermitian***, i.e.

$$\hat{H}_\theta \neq \hat{H}_\theta^\dagger \quad ; \tag{2.33}$$

and therefore the eigenvalues of $\hat{H}_\theta$ are complex. This is why we call this approach nonhermitian. Since the eigenvalues of $\hat{H}_\theta$, E_θ, are the same as the eigenvalues from the initial problem (2.1), they are ***independent of θ***. It can be shown that $\hat{H}_\theta$ can be acquired by a similarity transformation of $\hat{H}$, which will be described in more detail in Subsection 2.2.5.

When the condition (2.28) is met, the boundary conditions (2.31) become

$$\varphi_\theta\left(x \to \pm\infty\right) = 0 \quad . \tag{2.34}$$

We are reminded of the bound state boundary conditions (1.77), encountered in Chapter 1. This similarity will allow us to solve the boundary value problem (2.30), (2.34) for a toy potential model analogously to solving the bound state boundary problem in Chapter 1.

2.2.4 Numerical Calculation

We will now find a numerical solution to the boundary value problem (2.30), (2.34) analogously to solving the boundary value problem (1.76)-(1.77), only this time with the complex variable $z = xe^{i\theta} \in \mathbb{C}$ instead of $x \in \mathbb{R}$. Doing so we arrive at the matrix eigenvalue problem

$$\boxed{\boldsymbol{\underline{\underline{H_\theta}}\,\vec{c}_\theta = E_\theta\,\vec{c}_\theta}} \quad ; \tag{2.35}$$

[1] It can be shown that it is possible for small enough θ with potentials which are analytic functions of z [37].

[2] The importance of the phase $e^{i\frac{\theta}{2}}$ will be clarified later in Subsection 2.2.5.

where

$$b_j(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{j\pi}{L}\left(x - \frac{L}{2}\right)\right) \quad ; \quad j \in \mathbb{N} \quad ; \quad L \in \mathbb{R}^+ \quad ; \tag{2.36}$$

$$c_{\theta j} = \langle b_j | \varphi_\theta \rangle \tag{2.37}$$

and

$$H_{\theta jj'} := \langle b_j | - \frac{\hbar^2}{2m} e^{-2i\theta} \partial_{xx} | b_{j'} \rangle + \langle b_j | V(xe^{i\theta}) | b_{j'} \rangle \quad . \tag{2.38}$$

$\underline{\underline{H_\theta}}$ is an infinite nonhermitian matrix and $\vec{c}$ an infinite arithmetical column vector. In numerical calculations basis set truncation will again be performed. We have thus converted the operator eigenvalue problem into a matrix eigenvalue problem of linear algebra. We will now find a numerical solution to (2.35) for the toy potential (1.73) in arbitrary units and, as in Chapter 1, setting

$$\hbar = 1 \quad ; \quad m = 1 \quad . \tag{2.39}$$

The following relations will be used when calculating the elements of $\underline{\underline{H_\theta}}$:

$$\langle b_j | V(xe^{i\theta}) | b_{j'} \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) V(xe^{i\theta}) b_{j'}(x) =$$

$$= \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, (0.5x^2 e^{2i\theta} - 0.8) \exp\left(-0.1x^2 e^{2i\theta}\right) b_j(x) b_{j'}(x) \quad ; \tag{2.40}$$

$$\langle b_j | - \frac{\hbar^2}{2m} e^{-2i\theta} \partial_{xx} | b_{j'} \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) \left(-\frac{\hbar^2}{2m} e^{-2i\theta} \partial_{xx}\right) b_{j'}(x) =$$

$$= \frac{\hbar^2}{2m} \frac{(j')^2 \pi^2}{L^2} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x \, b_j(x) b_{j'}(x) = \frac{\hbar^2}{2m} \frac{(j')^2 \pi^2}{L^2} \delta_{jj'} \quad . \tag{2.41}$$

The basis set was truncated to include only its first 400 functions. The integration was done numerically with step size of $\mathrm{d}x = \frac{L}{10^6}$ and setting $L = 50$. The eigenvalue problem was then solved using the Eigen [16] package for C++.

The larger value of θ we use, the more resonances we can observe, but the less numerically stable our calculation is. As we will see, the ***bound state and resonance eigenvalues of $\hat{H}_\theta$ are in theory not dependent on θ***, but due to approximations used in our numerical model our calculated values of E_θ to a small degree are. The calculations were done using values of θ of 0.1, 0.2, 0,3 and 0.4 to illustrate this fact.

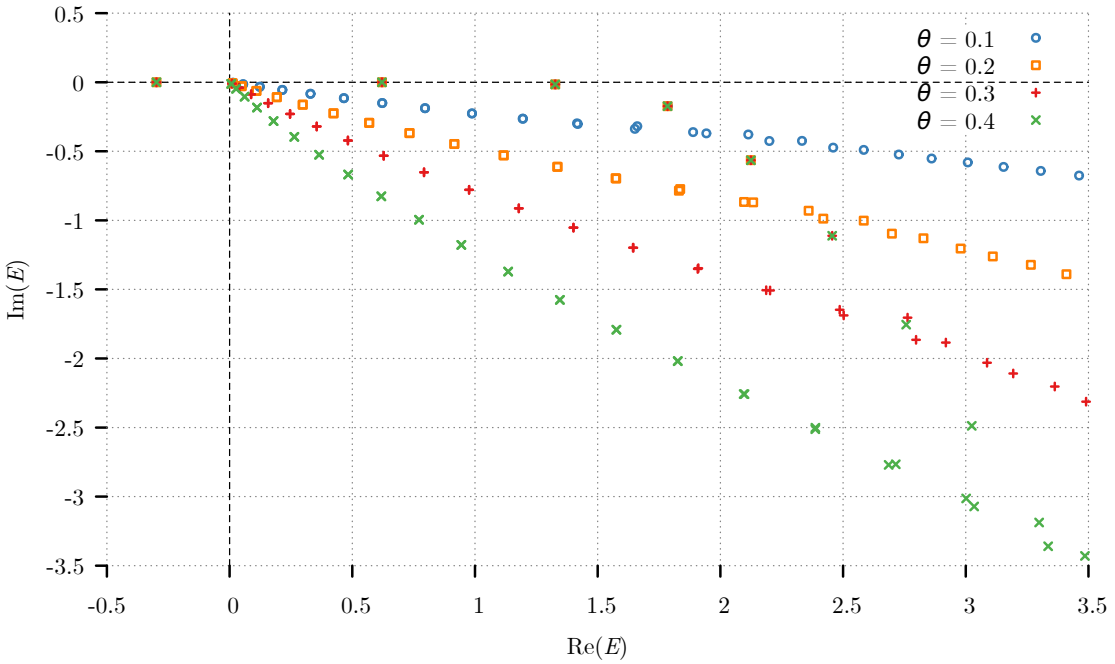

Figure 2.1: Resulting eigenvalues of $\hat{H}_\theta$ for different values of θ, composed of a rotated continuum, an eigenvalue corresponding to the bound state and the resonance eigenvalues. We see that for larger values of θ more resonance energies are visible and that their values nearly, but not perfectly, overlap for different values of θ. The just calculated resonances arise due to presence of the potential barriers, i.e. due to shape of the potential. We call them thus ***shape type resonances***.

Table 2.1: Resulting eigenvalues of $\hat{H}_\theta$ for the ground state and the first seven resonances. We notice that the eigenvalue E_0 is the same as the bound state energy in calculated in Chapter 1 and that the real parts of E_1, E_2 correspond to the peaks in transmission probability observed in Chapter 1, plotted in Figures 1.3-1.4.

	Re(E)	Im(E)
E_0	-0.29796	$2.22601 \cdot 10^{-14}$
E_1	0.62097	$-5.82666 \cdot 10^{-5}$
E_2	1.32720	-0.01545
E_3	1.78458	-0.17375
E_4	2.12442	-0.56480
E_5	2.45549	-1.11153
E_6	2.75722	-1.75551
E_7	3.02434	-2.48790

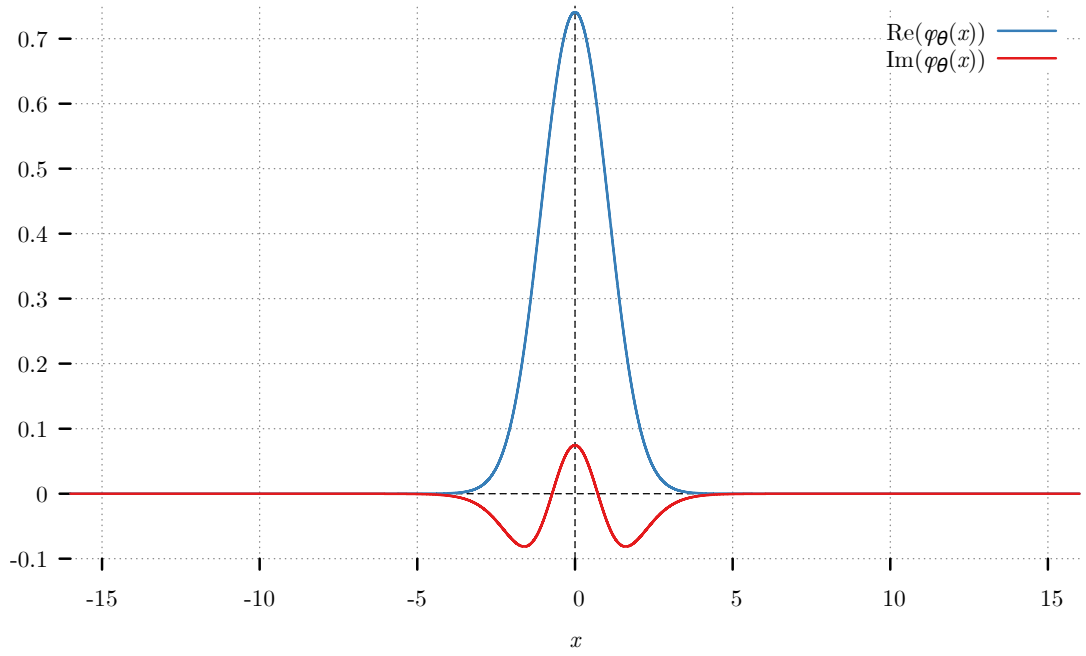

Figure 2.2: Real and imaginary parts of the the bound state with $E = E_0$, $\theta = 0.2$.

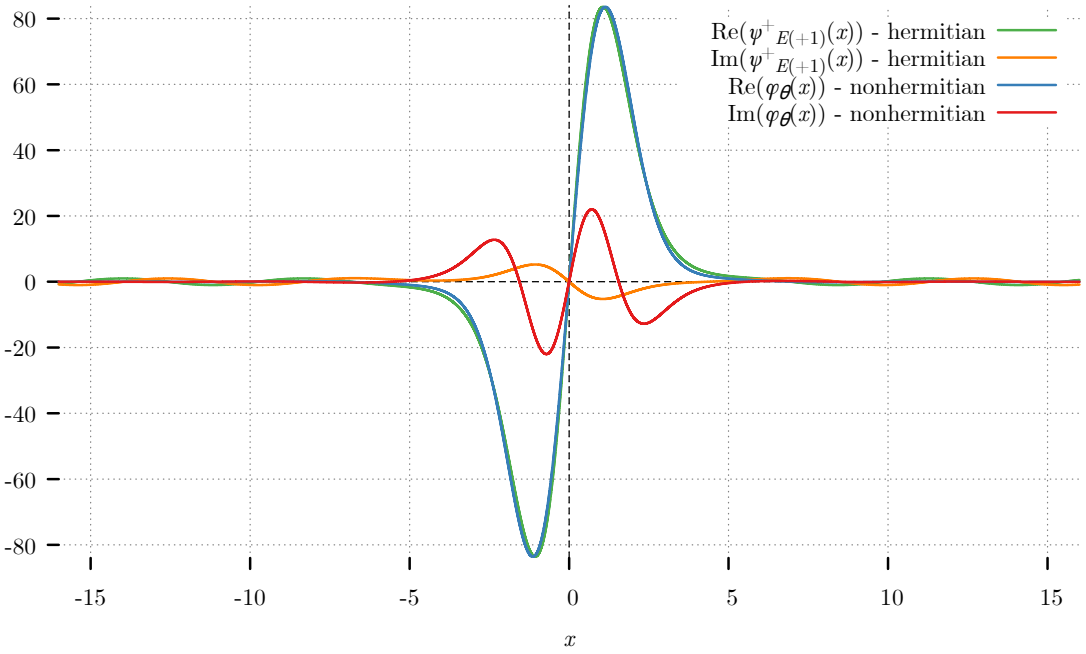

Figure 2.3: The first resonance wavefunction with $E = E_1$, $\theta = 0.2$ overlaid with the eigenfunction of $\hat{H}$ for $E = 0.62097$ calculated in Chapter 1.

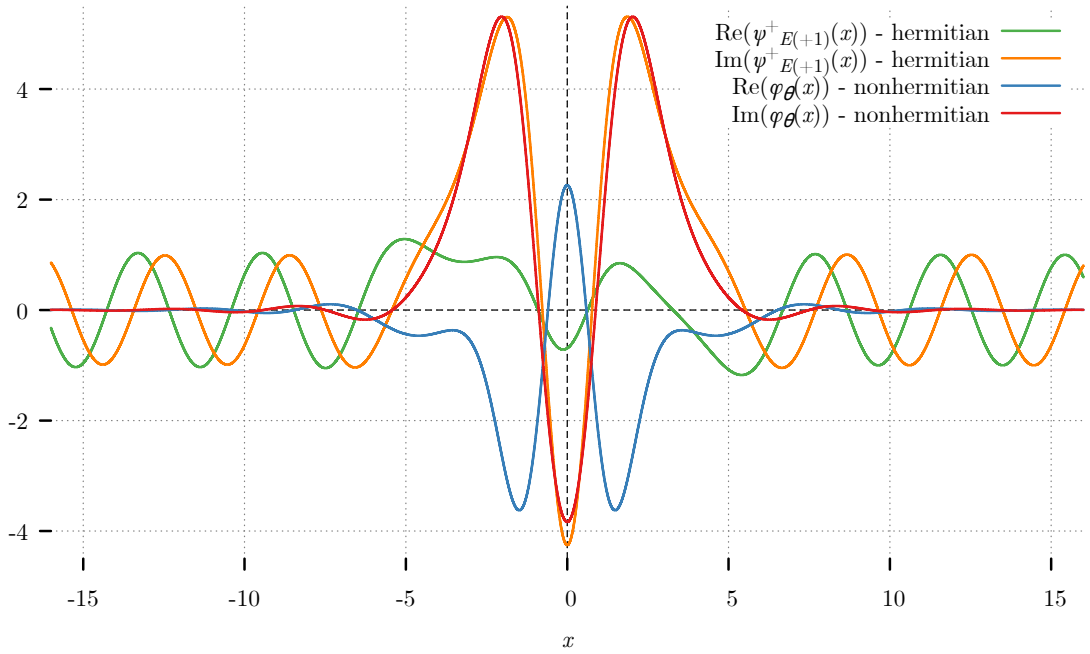

Figure 2.4: The second resonance wavefunction with $E = E_2$, $\theta = 0.2$ overlaid with the eigenfunction of $\hat{H}$ for $E = 1.32720$ calculated in Chapter 1.

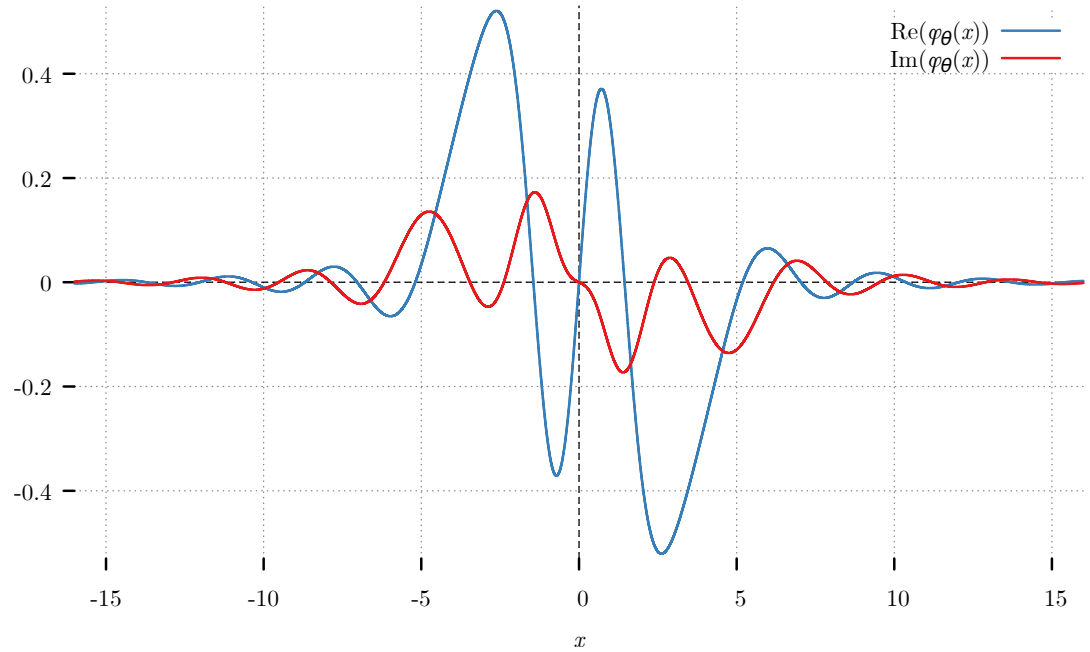

Figure 2.5: Real and imaginary parts of the third resonance wavefunction with $E = E_3$, $\theta = 0.2$.

Notice that the bound state as well as all the resonances are well contained in the interaction region $(-\frac{L}{2}, \frac{L}{2})$. The nodal structure of each resonance closely resembles the nodal structure of corresponding bound states of the LHO.

When comparing these results with the resonance wave functions obtained in Chapter 1 using methods of HQM, we see that the functions nearly overlap. This gives us confidence that the resonances defined as a special case of Gamow-Siegert states indeed describe the resonance phenomenon observed in Chapter 1. The reason these wave functions don't match perfectly is the interference by the other resonances in the hermitian case.

2.2.5 CS Operator

In this subsection we will define an make use of the so-called CS operator, which will let us formally implement complex scaling. Let ψ be an eigenfunction of $\hat{H}$, we then define the CS operator $\hat{S}_\theta : C^\infty(\mathbb{R}, \mathbb{C}) \to \mathcal{H}$ by the following relation:

$$\forall x \in \mathbb{R} \quad ; \quad (\hat{S}_\theta \psi)(x) = \psi(xe^{i\theta})e^{i\frac{\theta}{2}} = \varphi_\theta(x) \quad . \tag{2.42}$$

For small values of θ we can use the approximation

$$\psi(xe^{i\theta}) = \psi(x(1+i\theta))e^{i\frac{\theta}{2}} = \tag{2.43}$$

$$= (\psi(x) + \psi'(x)xi\theta)e^{i\frac{\theta}{2}} + o(\theta^2) = (1 + ix\theta\partial_x)e^{\frac{i}{2}\theta}\psi(x) + o(\theta^2) \quad . \tag{2.44}$$

Therefore, for infinitesimal $\mathrm{d}\theta$ we can write

$$\hat{S}_{\mathrm{d}\theta} = \hat{I} + ix\mathrm{d}\theta\partial_x \quad . \tag{2.45}$$

The finite complex rotation $\hat{S}_\theta$ can be obtained by repeated applications of the infinitesimal complex rotation $\hat{S}_{\mathrm{d}\theta}$, i.e.

$$\hat{S}_\theta = \hat{S}^n_{\mathrm{d}\theta} \quad ; \quad n \in \mathbb{N} \quad ; \tag{2.46}$$

$$\forall x \in \mathbb{R} \quad ; \quad \psi(xe^{ni\mathrm{d}\theta}) = (1 + ix\mathrm{d}\theta\partial_x)^n\psi(x) \quad . \tag{2.47}$$

Let $\mathrm{d}\theta = \frac{\theta}{n}$ and $n \to +\infty$, then

$$\boldsymbol{\hat{S}_\theta = \lim_{n\to+\infty}(\hat{I} + ix\mathrm{d}\theta\partial_x)^n e^{i\frac{\theta}{2}} = e^{ix\theta\partial_x}e^{i\frac{\theta}{2}}} \quad . \tag{2.48}$$

Let us now convert the eigenproblem (2.1) into a complex rotated eigenproblem:

$$\begin{aligned} \hat{H}\psi(x) &= E\psi(x) \quad \Big| \hat{S}_\theta \cdot \\ \hat{S}_\theta\hat{H}\hat{S}_\theta^{-1}\hat{S}_\theta\psi(x) &= E(\hat{S}_\theta\psi)(x) \\ \hat{H}_\theta\varphi_\theta(x) &= E\varphi_\theta(x) \quad ; \end{aligned} \tag{2.49}$$

where $\hat{H}_\theta$ is the previously encountered complex rotated Hamiltonian

$$\hat{H}_\theta = -\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta}) \quad ; \tag{2.50}$$

and

$$\hat{S}_\theta^{-1} = e^{-ix\theta\partial_x}e^{-i\frac{\theta}{2}} = \hat{S}_{-\theta} \quad . \tag{2.51}$$

This shows us that

$$\hat{H}_\theta = \hat{S}_\theta^{-1} \hat{H} \hat{S}_\theta \quad . \tag{2.52}$$

Proving that $\hat{H}$ and $\hat{H}_\theta$ are similar operators.

It can also be shown that the operator $\hat{S}_\theta$ is nonunitary [29], i.e.

$$\hat{S}_\theta^\dagger \neq \hat{S}_\theta^{-1} \quad . \tag{2.53}$$

The operator $\hat{H}_\theta$ is, therefore, nonhermitian, i.e.

$$\hat{H}_\theta \neq \hat{H}_\theta^\dagger \quad . \tag{2.54}$$

We shall now make a brief mathematical interlude, which will give us the necessary tools to better formally describe resonances and to introduce their normalization and closure.

2.2.6 Scalar Product, Orthonormality and Closure in Nonhermitian Quantum Mechanics - Matrix Formulation

For easier handling of the complex rotated eigenfunctions of $\hat{H}_\theta$, we need orthonormality and closure to be well defined. We will first introduce these concepts in the language of matrices. This will prove useful when constructing their wave function formulations. Let $N \in \mathbb{N}$ and $\underline{\underline{H}} \in \mathbb{C}^{N,N}$. We can express the eigenvalue problem of $\underline{\underline{H}}$ as

$$\det\Big(\underline{\underline{H}} - E\underline{\underline{I}}\Big) = 0 \quad ; \tag{2.55}$$

where $\underline{\underline{I}} \in \mathbb{C}^{N,N}$ is a unit matrix.

Assuming N distinct eigenvalues E_j (which is the generic case)

$$\forall j \in \{1, 2, \ldots, N\} \quad ; \quad \underline{\underline{H}}\, \vec{c}_j^{\,R} = E_j\, \vec{c}_j^{\,R} \quad ; \tag{2.56}$$

where $\vec{c}_j^{\,R}$ are the right eigenvectors of $\underline{\underline{H}}$. Let us now investigate the eigenvalue problem of the transposed matrix $\underline{\underline{H}}^\intercal$

$$\underline{\underline{H}}^\intercal \vec{d}_{\,j} = E_j\, \vec{d}_{\,j} \tag{2.57}$$

$$\vec{d}_{\,j}^{\,\intercal}\, \underline{\underline{H}} = E_j\, \vec{d}_{\,j}^{\,\intercal} \quad . \tag{2.58}$$

Therefore,

$$\vec{d}_{\,j} = \vec{c}_j^{\,L} \quad ; \tag{2.59}$$

where $\vec{c}_j^{\,L}$ are the left eigenvectors of $\underline{\underline{H}}$. Consequently

$$(\vec{c}_j^{\,L})^\intercal\, \underline{\underline{H}} = E_j (\vec{c}_j^{\,L})^\intercal \quad ; \tag{2.60}$$

$$\underline{\underline{H}}^\intercal\, \vec{c}_j^{\,L} = E_j\, \vec{c}_j^{\,L} \quad . \tag{2.61}$$

Both vectors $\vec{c}_j^{\,L}$ and $\vec{c}_j^{\,R}$ make up bases of the vector space $\mathbb{C}^N$.

C-product. Let $j, j' \in \{1, 2, \ldots, N\}$. Then we define C-product of $\vec{c}_{j'}$ and $\vec{c}_j$ as

$$(\vec{c}_{j'} | \vec{c}_j) \coloneqq (\vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j \quad . \tag{2.62}$$

Note that C-product is not positively definite and thus is not an actual scalar product for the vector space $\mathbb{C}^N$.

Turnover rule. *Let* $\vec{a}, \vec{b} \in \mathbb{C}^N$. *Then*

$$\vec{a}^\intercal \underline{\underline{H}} \vec{b} = (\underline{\underline{H}}^\intercal \vec{a})^\intercal \vec{b} \quad . \tag{2.63}$$

Proof. Follows directly from properties of transposed matrices. □

C-orthogonality relations. *Let* $j, j' \in \{1, 2, \ldots, N\}$ *and* $j \neq j'$. *Then*

$$(\vec{c}_{j'} | \vec{c}_j) = 0 \quad . \tag{2.64}$$

Proof.

$$\begin{aligned} \underline{\underline{H}} \vec{c}^{\,R}_j &= E_j \vec{c}^{\,R}_j \quad \Big| (\vec{c}^{\,L}_{j'})^\intercal \cdot \\ E_j (\vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j &= (\vec{c}^{\,L}_{j'})^\intercal \underline{\underline{H}} \vec{c}^{\,R}_j = (\underline{\underline{H}}^\intercal \vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j = E_{j'} (\vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j \\ (E_j - E_{j'}) (\vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j &= 0 \quad . \end{aligned}$$

$E_j \neq E_{j'}$, and therefore

$$(\vec{c}^{\,L}_{j'})^\intercal \vec{c}^{\,R}_j = 0 \quad .$$

□

We can also infer that

$$(\vec{c}_j | \vec{c}_j) \neq 0 \quad . \tag{2.65}$$

Because otherwise $\vec{c}^{\,L}_j$ would be orthogonal to every vector in $\mathbb{C}^N$, and therefore a zero vector, which is not an eigenvector of $\underline{\underline{H}}$. This allows us to introduce

C-normalization. Normalization of eigenvectors of $\underline{\underline{H}}$ such that $\forall j \in \{1, 2, \ldots, N\}$

$$(\vec{c}_j | \vec{c}_j) = 1 \quad . \tag{2.66}$$

By combining C-orthogonality relations with C-normalization we get

C-orthonormality relations. *Let* $j, j' \in \{1, 2, \ldots, N\}$. *Then*

$$(\vec{c}_{j'} | \vec{c}_j) = \delta_{j'j} \quad . \tag{2.67}$$

C-closure.

$$\sum_{j=1}^{N} \vec{c}^{\,R}_j (\vec{c}^{\,L}_j)^\intercal = \underline{\underline{I}} \quad . \tag{2.68}$$

Proof. Let $\vec{a} \in \mathbb{C}^N$. Since vectors $\vec{c}_j^{\,R}$ make up a basis of $\mathbb{C}^N$, there exist coefficients $\alpha_1, \alpha_2, \ldots, \alpha_N \in \mathbb{C}$ such that

$$\vec{a} = \sum_{j=1}^{N} \alpha_j \vec{c}_j^{\,R} \quad .$$

Therefore,

$$\sum_{j=1}^{N} \vec{c}_j^{\,R} (\vec{c}_j^{\,L})^{\intercal} \vec{a} = \sum_{j=1,k=1}^{N} \alpha_k \vec{c}_j^{\,R} (\vec{c}_j^{\,L})^{\intercal} \vec{c}_j^{\,R} = \sum_{j=1,k=1}^{N} \alpha_k \delta_{jk} \vec{c}_j^{\,R} = \sum_{j=1}^{N} \alpha_j \vec{c}_j^{\,R} = \vec{a} \quad .$$

□

Special Cases:

a) Matrix $\underline{\underline{H}}$ is hermitian, i.e. $\underline{\underline{H}} = \underline{\underline{H}}^{\dagger}$. Equation (2.61) can then be modified in the following way:

$$\underline{\underline{H}} \vec{c}_j^{\,R} = E_j \vec{c}_j^{\,R} \tag{2.69}$$

$$\underline{\underline{H}}^{\intercal} \vec{c}_j^{\,L} = E_j \vec{c}_j^{\,L} \quad \Big|^{*} \tag{2.70}$$

$$\underline{\underline{H}}^{\dagger} (\vec{c}_j^{\,L})^{*} = E_j (\vec{c}_j^{\,L})^{*} \quad ; \tag{2.71}$$

and therefore

$$\vec{c}_j^{\,L} = (\vec{c}_j^{\,R})^{*} \text{ (for the same normalization)} \quad . \tag{2.72}$$

Lets now denote $\vec{c}_j := \vec{c}_j^{\,R}$, and therefore also $\vec{c}_j^{\,*} = \vec{c}_j^{\,L}$. Orthonormality and closure can then be expressed as

$$(\vec{c}_{j'}^{\,*})^{\intercal} \vec{c}_j = \delta_{jj'} \quad ; \tag{2.73}$$

$$\sum_{j=0}^{N} \vec{c}_j (\vec{c}_j^{\,*})^{\intercal} = \underline{\underline{I}} \quad . \tag{2.74}$$

This situations occurs in the standard HQM, where the Hamiltonian $\hat{H}$ is hermitian.

b) Matrix $\underline{\underline{H}}$ is symmetrical and nonhermitian, i.e. $\underline{\underline{H}} = \underline{\underline{H}}^{\intercal} \neq \underline{\underline{H}}^{\dagger}$. Therefore,

$$\vec{c}_j^{\,R} = \vec{c}_j^{\,L} =: \vec{c}_j \quad . \tag{2.75}$$

Orthonormality and closure can then be expressed as

$$\vec{c}_{j'}^{\,\intercal} \vec{c}_j = \delta_{j'j} \quad ; \tag{2.76}$$

$$\sum_{j} \vec{c}_j \vec{c}_j^{\,\intercal} = \underline{\underline{I}} \quad . \tag{2.77}$$

This situation occurs in NHQM, where the complex rotated Hamiltonian $\hat{H}_\theta$ defined in (2.32) is nonhermitian. We can see that orthonormality and closure written in this form ***do not contain complex conjugation***, this is an important difference from the hermitian forms (2.73)-(2.74).

Degeneracies

Degeneracies correspond to the so-called ***exceptional points***, for adequate description of which an even more general formulation is required. They will be demonstrated on 2-by-2 matrices later in Chapter 3.

2.2.7 Scalar Product, Orthonormality and Closure in Nonhermitian Quantum Mechanics - Wave Function Formulation

We shall now translate these concepts into the language of eigenstates of the complex rotated Hamiltonian $\hat{H}_\theta$, defined in (2.32). Let $\forall j \in \mathbb{N}, \varphi_{\theta,j} \in C^\infty(\mathbb{R},\mathbb{C})$ be distinct eigenvectors of $\hat{H}_\theta$ and $\{b_n(x)\}_{n=1}^\infty \subset C^\infty(\mathbb{R},\mathbb{R})$ a complete basis set of $C^\infty(\mathbb{R},\mathbb{C})$. Hamiltonian matrix elements of $\hat{H}_\theta$ can then be calculated as

$$H_{\theta nn'} = \int_{-\infty}^{+\infty} b_n(x)\hat{H}_\theta b_{n'}(x)\,\mathrm{d}x, \quad \forall n,n' \in \mathbb{N} \tag{2.78}$$

and its eigenvectors as

$$\varphi_j(x) = \sum_n c_j^n b_n(x) \quad ; \tag{2.79}$$

where

$$\forall j \in \mathbb{N} \quad ; \quad c_j \in \mathbb{C} \quad . \tag{2.80}$$

The expression (2.78) does not contain complex conjugation, since $\forall n \in \mathbb{N}, \forall x \in \mathbb{R}, b_n(x) \in \mathbb{R}$. From the characteristics of the operator $\hat{H}_\theta$, we see that the matrix $\underline{\underline{H_\theta}} \in \mathbb{C}^{\infty,\infty}$, made up of elements (2.78), is symmetric.

Next we translate into the language of wave functions the C-product defined in the previous subsection in (2.62).

C-product. Let $j,j' \in \mathbb{N}$. Then we define C-product of vectors $\varphi_{\theta j}$ and $\varphi_{\theta j'}$ as

$$(\varphi_{\theta j}|\varphi_{\theta j'}) := \int_{\mathbb{R}} \mathrm{d}x\, \varphi_{\theta j}(x)\varphi_{\theta j'}(x) = (\varphi_{\theta j'}|\varphi_{\theta j}) \tag{2.81}$$

C-product is the scalar product in NHQM. Since $(\varphi_{\theta j}|\varphi_{\theta j})$ can be complex valued, C-product again is not positively semidefinitive and as such not an actual scalar product for the vector space $C^\infty(\mathbb{R},\mathbb{C})$.

In what follows we will truncate the basis $\{b_n(x)\}_{n=1}^\infty$ to include only its first $N \in \mathbb{N}$ functions. This will make $\underline{\underline{H_\theta}}$ an $N \times N$ matrix, which will let us make use of the developments made in Subsection 2.2.7.

Turnover rule. *Let* $j,j' \in \{1,2,\ldots,N\}$. *Then*

$$(\varphi_{\theta j}|\hat{H}_\theta|\varphi_{\theta j'}) = (\hat{H}_\theta\varphi_{\theta j}|\varphi_{\theta j'}) \tag{2.82}$$

Proof. Follows directly from the matrix turnover rule (2.63) proven in the previous subsection. □

C-orthogonality relations. *Let* $j, j' \in \{1, 2, \ldots, N\}$ *and* $j \neq j'$. *Then*

$$(\varphi_{\theta,j}|\varphi_{\theta,j'}) = 0 \quad . \tag{2.83}$$

Proof. Follows directly from the matrix C-orthogonality relations (2.64) proven in the previous subsection. □

C-normalization. Normalization of eigenvectors of $\hat{H}_\theta$ such that $\forall j \in \{1, 2, \ldots, N\}$

$$(\varphi_{\theta j}|\varphi_{\theta j}) = 1 \tag{2.84}$$

By combining C-orthogonality relations with C-normalization we get

C-orthonormality relations. *Let* $j, j' \in \{1, 2, \ldots, N\}$. *Then*

$$(\varphi_{\theta,j}|\varphi_{\theta,j'}) = \delta_{jj'} \quad . \tag{2.85}$$

C-closure. *Let* $x, x' \in \mathbb{R}$. *Then*

$$\sum_{j=1}^{N} \varphi_{\theta j}(x)\varphi_{\theta j}(x') = \delta(x - x') \quad . \tag{2.86}$$

Proof. Let $f(x) = \delta(x - x')$. Since $\{b_n(x)\}_{n=1}^N$ is a complete basis set, there exist coefficients $\{f_n\}_{n=1}^N \in \mathbb{C}$ such that

$$f(x) = \sum_{n=1}^{N} f_n b_n(x) \quad ;$$
$$f_n = \int_{-\infty}^{+\infty} b_n(x) f(x)\, \mathrm{d}x = \int_{-\infty}^{+\infty} b_n(x)\delta(x - x')\, \mathrm{d}x = b_n(x') \quad .$$

Therefore,

$$f(x) = \sum_{n=1}^{N} b_n(x) b_n(x') \quad .$$

Using the closure property of eigenvectors of $\underline{\underline{H_\theta}} \in \mathbb{C}^{N,N}$

$$\sum_{j=1}^{N} c_j^n c_j^{n'} = \delta_{nn'} \quad ;$$

we get

$$\sum_{j=1}^{N} \psi_j(x)\psi_j(x') = \sum_{j,n,n'} c_j^n b_n(x) c_j^{n'} b_{n'}(x') = \sum_{n=1}^{N} b_n(x) b_n(x') = f(x) = \delta(x - x') \quad .$$

□

2.2.8 The Independence of the C-product of the Angle of Complex Rotation

Let us now take a look at C-product of eigenvectors of $\hat{H}_\theta$, $\varphi_{\theta,1}, \varphi_{\theta,2}$, created by complex rotation of the eigenvectors of $\hat{H}$, ψ_1, ψ_2, by angle θ

$$\begin{aligned}(\varphi_{\theta,1}|\varphi_{\theta,2}) &= \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{i\theta}\psi_1(xe^{i\theta})\psi_2(xe^{i\theta}) = \\ &= \int_{-\infty}^{+\infty} \mathrm{d}(xe^{i\theta})\psi_1(xe^{i\theta})\psi_2(xe^{i\theta}) \quad . \end{aligned} \tag{2.87}$$

Theorem 2. *C-product is independent of the angle of complex rotation.*

Proof. Let ψ_1, ψ_2 be eigenvectors of $\hat{H}$ and $\varphi_{\theta,1}, \varphi_{\theta,2}$ eigenvectors of $\hat{H}_\theta$ created by complex rotation of ψ_1, ψ_2 by angle $\theta \in (0; 2\pi)$. We will construct an oriented closed loop γ such that

$$(\varphi_{\theta,1}|\varphi_{\theta,2}) - (\varphi_{\theta',1}|\varphi_{\theta',2}) = \int_\gamma \mathrm{d}z\, \psi_1(z)\psi_2(z) \quad \text{(contour integration)} \quad .$$

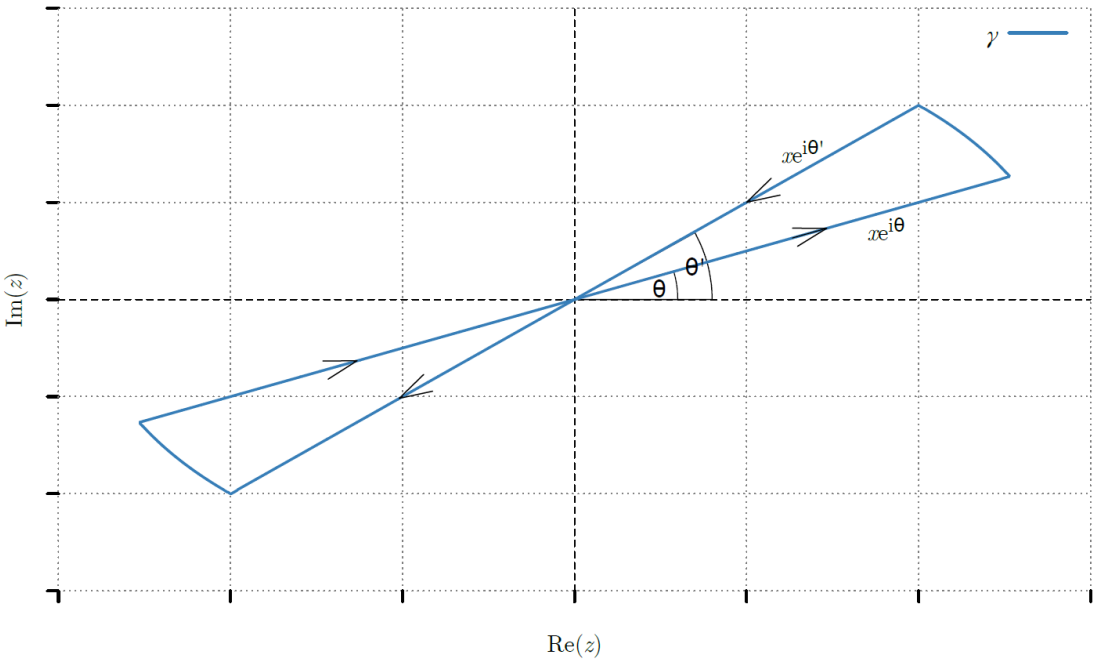

Figure 2.6: The closed loop created by connecting the two complex rotated contours $xe^{i\theta}$ and $xe^{i\theta'}$. We choose the integration direction to be counterclockwise.

Since the complex function $\psi_1(z)\psi_2(z)$ is analytic on the, simply connected, interior of γ, then, according to Cauchy's integral theorem [2],

$$\int_\gamma \mathrm{d}z\, \psi_1(z)\psi_2(z) = 0 \quad .$$

Therefore,

$$\forall \theta, \theta' \in \left(0, \frac{\pi}{2}\right) \quad ; \quad (\varphi_{\theta,1}|\varphi_{\theta,2}) = (\varphi_{\theta',1}|\varphi_{\theta',2}) \quad .$$

□

In further calculations, we will use basis functions $b_n(x)$, which are even for even n and odd for odd n, i.e.

$$\forall n \in \{1, 2, \ldots, N\} \quad ; \quad \forall x \in \mathbb{R} \quad ; \quad b_n(-x) = (-1)^n b_n(x) \quad . \tag{2.88}$$

For a symmetric potential then

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, b_n(x) \hat{H}_\theta b_{n'}(x) \neq 0 \tag{2.89}$$

only for n, n' with the same parity. The matrix $\underline{\underline{H_\theta}}$ can, therefore, be written as

$$\underline{\underline{H_\theta}} = \begin{pmatrix} n_{\text{even}} & 0 \\ 0 & n_{\text{odd}} \end{pmatrix} \quad . \tag{2.90}$$

Vectors $\varphi_{j,\theta}$ can thus also be divided into even and odd ones. Using this knowledge, we can rewrite the orthonormality relations (2.85) as

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \varphi_{\alpha,\theta}(x) \varphi_{\alpha',\theta}(x) = \delta_{\alpha\alpha'} \quad ; \tag{2.91}$$

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \varphi_{\alpha,\theta}(x) \varphi_{E\nu,\theta}(x) = 0 \quad ; \tag{2.92}$$

$$\int_{-\infty}^{+\infty} \mathrm{d}x \, \varphi_{E\nu,\theta}(x) \varphi_{E'\nu,\theta}(x) = \delta_{\nu\nu'} \delta(E - E') \quad ; \tag{2.93}$$

where $\nu = 0$ for even and $\nu = 1$ for odd eigenvectors of $\hat{H}_\theta$. In this notation, the vectors $\varphi_{\alpha,\theta}$ represent bound states and resonances, and the vectors $\varphi_{E\nu,\theta}$ represent the complex rotated continuum. The closure property (2.86) can, with such a basis, be rewritten as

$$\sum_\alpha \varphi_{\alpha,\theta}(x) \varphi_{\alpha,\theta}(x) + \sum_\nu \int_\gamma \mathrm{d}E \, \psi_{E\nu,\theta}(x) \varphi_{E\nu,\theta}(x') = \delta(x - x') \quad . \tag{2.94}$$

2.2.9 Zeldovich C-product

To guarantee that functions $\varphi_{j,\theta}$ are integrable even for small angles, we can expand the C-product by multiplying it by the expression $\lim_{\epsilon \to 0^+} e^{-\epsilon x^2}$, creating the

Zeldovich C-Product. We define Zeldovich C-product of vectors ψ_1 and ψ_2 as

$$(\psi_1|\psi_2)_Z \coloneqq \lim_{\epsilon \to 0^+} \int_{\mathbb{R}} \mathrm{d}x \, \psi_1(x) \psi_2(x) e^{-\epsilon x^2} = (\psi_2|\psi_1)_Z \quad . \tag{2.95}$$

Let us now consider the Zeldovich C-product of vectors $\varphi_{\theta,1}, \varphi_{\theta,2}$ created by complex rotation of vectors ψ_1, ψ_2 by angle θ

$$(\varphi_{\theta,1}|\varphi_{\theta,2})_Z = \lim_{\epsilon\to 0^+} \int_{-\infty}^{+\infty} \mathrm{d}(xe^{i\theta})\psi_1(xe^{i\theta})\psi_2(xe^{i\theta}) \exp\left(-\epsilon(xe^{i\theta})^2\right) \quad ; \tag{2.96}$$

where

$$\exp\left(-\epsilon(xe^{i\theta})^2\right) = \exp\left(-\epsilon x^2\cos(2\theta)\right)\exp\left(-\epsilon x^2 i\sin(2\theta)\right) \quad ; \tag{2.97}$$

and thus

$$\forall\theta \in [0, \frac{\pi}{4}] \quad ; \quad \lim_{x\to\pm\infty} \exp\left(-\epsilon x^2\cos(2\theta)\right) = 0 \quad . \tag{2.98}$$

Therefore, ***$(\varphi_{\theta,1}|\varphi_{2,\theta})_Z$ is well defined even for small values of θ***. Using the same contour integration argument as in the proof of Theorem 2, we see that the value of the standard C-product (2.81) and the Zeldovich C-product (2.95) is identical for all pairs of vectors, whose C-product is well defined.

2.2.10 Complex Scaled Scattering Theory

We will now use the mathematical developments made in the previous subsections to derive a formula for the so-called ***Breit-Wigner profiles***, which will enable us to isolate the peaks in transmission probability caused by individual resonances. The transmission coefficient $T(E)$ is a physically observable quantity and thus has the same value no matter if it is calculated using methods of HQM or NHQM. The hermitian formula for $T(E)$, (1.56), can be generalized in NHQM as [38]

$$T(E) = 1 - 2\pi i(\phi^\theta_{E(+1)}|\hat{V}_\theta + \hat{V}_\theta\frac{1}{E-\hat{H}_\theta}\hat{V}_\theta|\phi^\theta_{E(+1)}) \quad ; \tag{2.99}$$

where

$$\phi^\theta_{E(+1)} \coloneqq \hat{S}_\theta\phi_{E(+1)}(x) = e^{i\frac{\theta}{2}}\phi_{E(+1)}(xe^{i\theta}) \quad ; \tag{2.100}$$

$$V_\theta \coloneqq V(xe^{i\theta}) \tag{2.101}$$

and $\phi_{E(+1)}(x)$ are the eigenvectors of the free particle Hamiltonian $\hat{H}_0$, defined in (1.7). Let ξ^θ_j be eigenvectors of the complex rotated Hamiltonian $\hat{H}_\theta$, then [29]

$$\hat{H}_\theta|\xi^\theta_j) = \mathcal{E}^\theta_j|\xi^\theta_j) \quad ; \tag{2.102}$$

$$\frac{1}{E-\hat{H}_\theta} = \sum_j \frac{|\xi^\theta_j)(\xi^\theta_j|}{E-\mathcal{E}^\theta_j} \quad . \tag{2.103}$$

We call the expression (2.103) the spectral representation of the nonhermitian Green operator. It is well defined since

$$\forall j\in\mathbb{N}, \mathrm{Im}[E_j] \neq 0 \Rightarrow \forall j\in\mathbb{N}, E\neq E_j \Rightarrow E-\hat{H}_\theta \neq 0 \quad . \tag{2.104}$$

As we can see, the nonhermitian formula (2.99) eliminates the singularity in the denominator without having to add the factor $i0_\pm$, seen in (1.56). This in practice makes the calculation significantly easier [38].

Since $V(x \to \pm\infty) = 0$, we can again use contour integration to get

$$\begin{aligned}
&\left(\phi^{\theta}_{E(+1)} \left|V_\theta\right| \phi^{\theta}_{E(+1)}\right) = \left\langle \phi_{E(+1)} \right| V \left| \phi_{E(+1)} \right\rangle = \\
&= \int_{-\infty}^{+\infty} \mathrm{d}x \sqrt{\frac{m}{2\pi\hbar^2 k}} e^{-kx} V(x) \sqrt{\frac{m}{2\pi\hbar^2 k}} e^{ikx} = \\
&= \int_{-\infty}^{+\infty} \mathrm{d}x\, V(xe^{i\theta}) e^{i\frac{\theta}{2}} \sqrt{\frac{m}{2\pi\hbar^2 k}} \exp\left(ikxe^{i\theta}\right) e^{i\frac{\theta}{2}} \sqrt{\frac{m}{2\pi\hbar^2 k}} \exp\left(-ikxe^{i\theta}\right) \quad ; \qquad (2.105)
\end{aligned}$$

and therefore

$$\begin{aligned}
&T(E) = \qquad (2.106)\\
&= 1 - 2\pi i \int_{-\infty}^{+\infty} \mathrm{d}x\, V(xe^{i\theta}) e^{i\frac{\theta}{2}} \sqrt{\frac{m}{2\pi\hbar^2 k}} \exp\left(ikxe^{i\theta}\right) e^{i\frac{\theta}{2}} \sqrt{\frac{m}{2\pi\hbar^2 k}} \exp\left(-ikxe^{i\theta}\right) + \\
&- 2\pi i \sum_j \frac{(\phi^{\theta}_{E(+1)} | \hat{V}^{\theta}_j | \xi^{\theta}_j)(\xi^{\theta}_j | \hat{V}^{\theta}_j | \phi^{\theta}_{E(+1)})}{E - \mathcal{E}^{\theta}_j} \quad . \qquad (2.107)
\end{aligned}$$

We are summing the contributions of bound states, resonances and of the complex rotated continuum. (There the sum transforms into an integral.) The value of $T(E)$ is again independent of the angle θ. As we can see, the contribution of any given resonance or bound state j is

$$-2\pi i \frac{(\phi_{E(+1)} | \hat{V}_j | \xi_j)(\xi_j | \hat{V}_j | \phi_{E(+1)})}{E - \mathcal{E}_j} \quad . \qquad (2.108)$$

Let us now consider the situation, where the real positive energy of the incoming particle is close to a resonance energy E_j (not a bound state), i.e. $E \approx \mathcal{E}_j$. We can then make the following approximation:

$$T(E) \approx \frac{(\phi_{E(+1)} | \hat{V}_j | \xi_j)(\xi_j | \hat{V}_j | \phi_{E(+1)})}{E - \mathcal{E}_j} \approx \frac{-i\Gamma_j/2}{E - (E_j - \frac{i}{2}\Gamma_j)} \quad . \qquad (2.109)$$

$$\Rightarrow \boxed{|\boldsymbol{T(E)}|^2 \approx \frac{\boldsymbol{\Gamma_j^2/4}}{\boldsymbol{(E - \mathcal{E}_j)^2 + \Gamma_j^2/4}} =: |\boldsymbol{T^{(j)}_{\mathrm{BW}}(E)}|^2} \quad ; \qquad (2.110)$$

where

$$E_j =: \mathcal{E}_j - \frac{i}{2}\Gamma_j \quad ; \quad E_j, \Gamma_j \in \mathbb{R} \quad . \qquad (2.111)$$

These is the so-called ***Breit-Wigner profiles***. Since $E \in \mathbb{R}$, this approximation is only accurate for isolated resonances with $\Gamma_j \approx 0$. The transmission probability $|T(E)|^2$, as seen in Figure 1.2, is made up of Breit-Wigner profiles of overlapping resonances, see Figure 2.9 bellow.

2.2.11 Numerical Calculation - Breit-Wigner Profile

We will now make use of the previously calculated resonance energies, displayed in Table 2.1, by plotting the first four Breit-Wigner profiles and comparing them to the transmission probability calculated in Chapter 1, as seen in Figure 1.2.

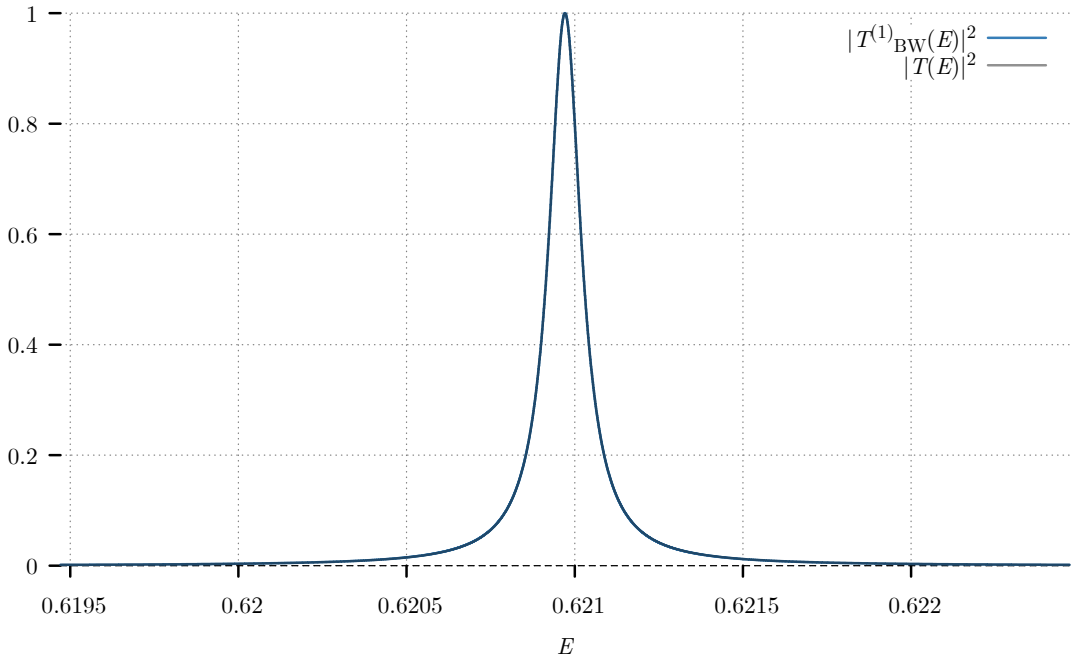

Figure 2.7: The Breit-Wigner profile for $j = 1$ overlaid with the hermitian calculation of the first peak in $|T(E)|^2$, seen in Figure 1.3. Notice that these plots match very closely. This is because of only very small interference of resonances other than the first one.

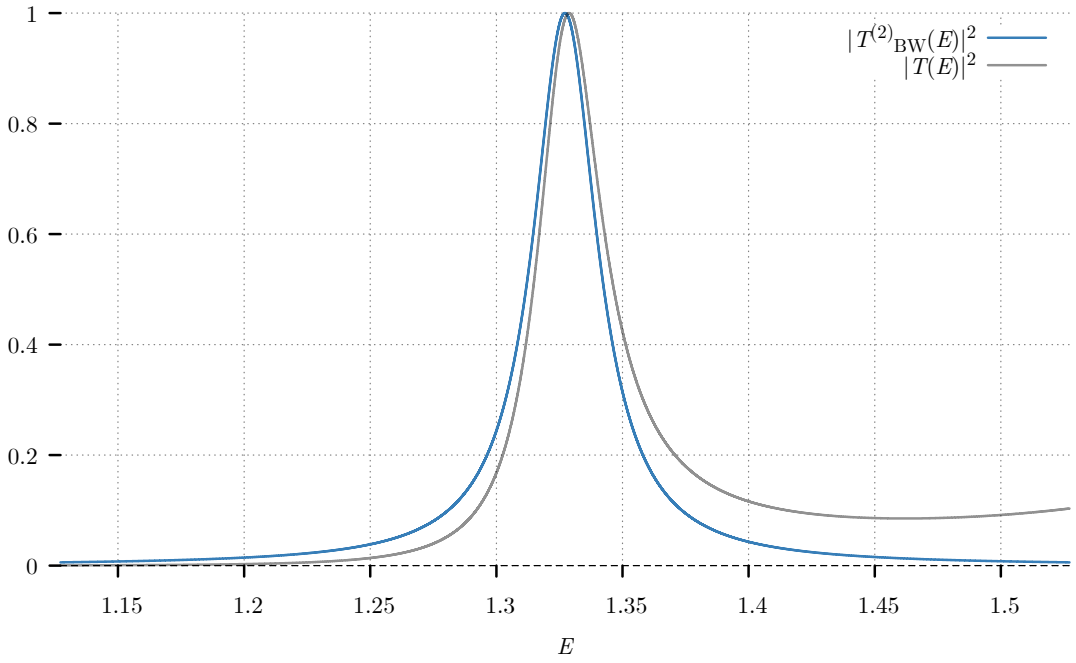

Figure 2.8: The Breit-Wigner profile for $j = 2$ overlaid with the hermitian calculation of the first peak in $|T(E)|^2$, seen in Figure 1.4. Notice that these plots match closely, however, to a lesser degree than in Figure 2.2.11. This is because of a slight interference of resonances other than the second one.

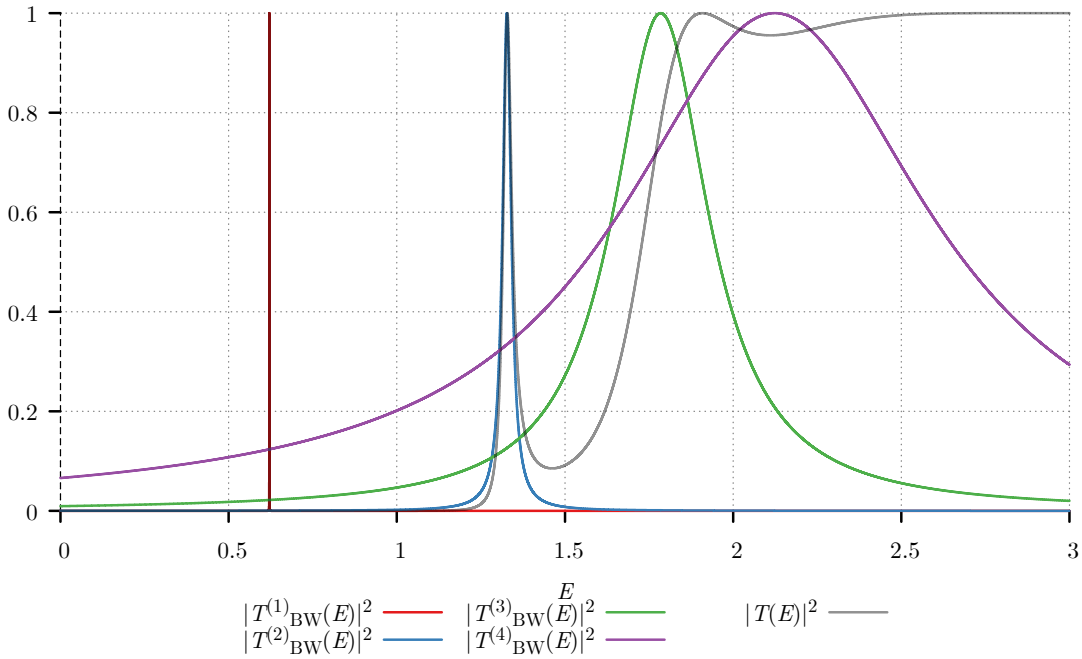

Figure 2.9: The hermitian calculation of the transmission probability from Figure 1.2 overlaid with the first 4 resonances. The first two peaks match closely with $|T(E)|^2$, the others less so, as the peaks get wider and the interference of other resonances larger.

2.2.12 Summary

In this section we have described the ***complex coordinate method*** and used it, along a numeric model, to solve the ***Siegert boundary value problem for resonances***. We have then established the concepts of the scalar product, orthonormality and closure in NHQM and used them to numerically calculate the ***Breit-Wigner profiles*** of the first four resonances.

The main advantage of CS lies in its wide applicability (multidimensional many electron systems, exceptional points in experiments [29]).

It does however also have two major disadvantages: *i)* It is not applicable to such potentials, which are not dilation analytic [37]. (This obstacle is overcome by means of the so called exterior complex scaling method [29].) *ii)* It is not applicable for the calculation of the anti bound states.

The open problems regarding CS include: *i)* The determination of the quantum mechanical expectation values (position, momentum, acceleration, spectra of high harmonic generation). *ii)* Finding a way of adequately describing wave packet dynamics.

2.3 Method of Siegert Pseudostates

2.3.1 Introduction

When using this method, we will be working with the original Gamow-Siegert states, established in Subsection 2.1.1, without modifying them to become square-integrable, as opposed to what we did when using complex scaling. For several decades after the invention of Gamow-Siegert states, at the hands of Gamow and Siegert [36], there were no clear ways of efficiently calculating them, and in particular of constructing an appropriate closure property and formulating the scattering theory in terms of these states. It was then Tolstikhin in the 1990s, whose illuminating insights have facilitated an enormous progress leading to an extremely elegant formulation of the nonhermitian scattering theory in terms of the Siegert pseudostates [42]. This powerful formalism of Tolstikhin is outlined below.

We define the Siegert pseudostates as finite basis representations of the Gamow-Siegert states. We will, therefore, be again solving the equation

$$\left(-\frac{\hbar^2}{2m}\partial_{xx} + V(x)\right)\psi(x) = E\psi(x) \quad ; \quad E \in \mathbb{C} \tag{2.112}$$

with the same Siegert type boundary conditions, defined in Subsection 2.1.1,

$$\psi\left(x \to -\infty\right) = C_- e^{-iKx} = C_- e^{-iK_1 x} e^{K_2 x} \quad ; \tag{2.113}$$

$$\psi\left(x \to +\infty\right) = C_+ e^{iKx} = C_+ e^{iK_1 x} e^{-K_2 x} \quad ; \tag{2.114}$$

where

$$C_-, C_+ \in \mathbb{C} \quad . \tag{2.115}$$

2.3.2 Basis Set Expansion

Let $a \in \mathbb{R}^+$ be large enough such that, thanks to the boundary conditions (2.113)-(2.114),

$$\psi(x > a) \approx C_+ e^{iKx} \quad ; \tag{2.116}$$

$$\psi(x < -a) \approx C_- e^{-iKx} \quad ; \tag{2.117}$$

which can be equivalently expressed as

$$(\partial_x \pm iK)\psi(x)\big|_{x=\mp a} = 0 \quad ; \tag{2.118}$$

and therefore

$$\psi'(\pm a) = \pm ik\psi(a) \quad . \tag{2.119}$$

Since we know the value of $\psi(x)$ for $x \in \mathbb{R} \setminus (-a, a)$ (and it diverges), we can limit ourselves to the region $x \in [-a, a]$. We will now expand our eigenfunctions using the Legendre basis

$$\{b_\nu(x)\}_{\nu=0}^{\infty} \quad ; \quad b_\nu(x) = \sqrt{\frac{2\nu+1}{2a}} P_\nu(\frac{x}{a}) \quad ; \tag{2.120}$$

where P_ν are the Legendre polynomials, derivatives of which are easily obtained using the recursive formula

$$\forall u \in \mathbb{R} \quad ; \quad \frac{u^2-1}{n}\frac{\mathrm{d}}{\mathrm{d}u}P_n(u) = (2n+1)uP_n(u) - P_{n-1}(u) \quad . \tag{2.121}$$

The expansion is possible for any function in $\mathrm{C}(\mathbb{R},\mathbb{C})$, unlike with the previously used particle-in-a-box basis set, where we could only expand functions vanishing at the ends of the interaction region $[-a,a]$. This is due to the Legendre basis possessing the closure property and being made up of functions that don't die out for $x = \pm a$. This basis is also orthonormal on the interval $[-a,a]$, which will be useful in later calculations. This allows us to write $\psi(x)$ as

$$\psi(x) = \sum_\nu c_\nu b_\nu(x) \quad . \tag{2.122}$$

Let us now perform the following operations on the Schrödinger Equation (2.112):

$$-\frac{\hbar^2}{2m}\partial_{xx}\psi(x) + V(x)\psi(x) = E\psi(x) \quad \Big| \int_{-a}^{a} \mathrm{d}x\, b_\nu(x) \tag{2.123}$$

$$\begin{aligned} &b_\nu(a)(-\frac{\hbar^2}{2m})\psi'(a) - b_\nu(-a)(-\frac{\hbar^2}{2m})\psi'(-a) + \frac{\hbar^2}{2m}\int_{-a}^{a}\mathrm{d}x\, b'_\nu(x)\psi'(x) + \\ &+ \int_{-a}^{a}\mathrm{d}x\, b_\nu(x)V(x)\psi(x) = E\int_{-a}^{a}\mathrm{d}x\, b_\nu(x)\psi(x) \end{aligned} \tag{2.124}$$

$$\begin{aligned} &-b_\nu(a)\frac{\hbar^2}{2m}ik\psi(a) - b_\nu(-a)(-\frac{\hbar^2}{2m})ik\psi(a)) + \frac{\hbar^2}{2m}\int_{-a}^{a}\mathrm{d}x\, b'_\nu(x)ik\psi(a) + \\ &+ \int_{-a}^{a}\mathrm{d}x\, b_\nu(x)V(x)\psi(x) = E\int_{-a}^{a}\mathrm{d}x\, b_\nu(x)\psi(x) + \\ &-\frac{\hbar^2}{2m}\sum_{\nu'}(b_\nu(a)b_{\nu'}(a) + b_\nu(-a)b_{\nu'}(-a))c_{\nu'} + \frac{\hbar^2}{2m}\sum_{\nu'}\int_{-a}^{a}\mathrm{d}x\, b'_\nu(x)b'_{\nu'}(x)c_{\nu'} + \\ &+ \sum_{\nu'}\int_{-a}^{a}\mathrm{d}x\, b_\nu(x)V(x)b_{\nu'}(x)c_{\nu'} = Ec_\nu \quad . \end{aligned} \tag{2.125}$$

We have thus transformed the eigenvalue problem (2.112)-(2.114) into an algebraic problem for coefficients c_ν. The system of equations obtained in this way can be, for more convenient handling, rewritten into the matrix formulation

$$\left(\underline{\underline{H}} - iK\underline{\underline{L}} - \frac{\hbar^2K^2}{2m}\underline{\underline{I}}\right)\vec{c} = \vec{0} \quad ; \tag{2.126}$$

where

$$H_{\nu\nu'} = \frac{\hbar^2}{2m}\int_{-a}^{a}\mathrm{d}x\, b'_\nu(x)b'_{\nu'}(x) + \int_{-a}^{a}\mathrm{d}x\, b_\nu(x)V(x)b_{\nu'}(x) \quad ; \tag{2.127}$$

$$L_{\nu\nu'} \coloneqq \frac{\hbar^2}{2m}(b_\nu(a)b_{\nu'}(a) + b_\nu(-a)b_{\nu'}(-a)) \quad . \tag{2.128}$$

This is a ***quadratic eigenvalue problem*** for the eigenvalues K and eigenvectors $\vec{c}$ that can be further simplified as

$$(\underline{\underline{A}} + \lambda \underline{\underline{B}} + \lambda^2 \underline{\underline{I}})\vec{c} = \vec{0} \quad ; \tag{2.129}$$

where

$$\underline{\underline{A}} := \frac{2m}{\hbar^2}\underline{\underline{H}} \quad ; \tag{2.130}$$

$$\underline{\underline{B}} := -\frac{2m}{\hbar^2}\underline{\underline{L}} \quad ; \quad \lambda := iK \quad . \tag{2.131}$$

The solution procedure for the eigenproblem (2.129) is not apriori obvious. It can however be transformed into a much more easily solvable linear eigenvalue problem by using the following notation (linearization):

$$\begin{pmatrix} \vec{c} \\ \tilde{\vec{c}} \end{pmatrix} := \begin{pmatrix} \vec{c} \\ \lambda \vec{c} \end{pmatrix} \quad . \tag{2.132}$$

The problem then becomes

$$\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{I}} \\ -\underline{\underline{A}} & -\underline{\underline{B}} \end{pmatrix} \begin{pmatrix} \vec{c} \\ \tilde{\vec{c}} \end{pmatrix} = \lambda \begin{pmatrix} \vec{c} \\ \tilde{\vec{c}} \end{pmatrix} \tag{2.133}$$

$$\begin{pmatrix} \underline{\underline{B}} & \underline{\underline{0}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{I}} \\ -\underline{\underline{A}} & -\underline{\underline{B}} \end{pmatrix} = \begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix}$$

$$\boxed{\begin{pmatrix} -\underline{\underline{\boldsymbol{A}}} & \underline{\underline{\boldsymbol{0}}} \\ \underline{\underline{\boldsymbol{0}}} & \underline{\underline{\boldsymbol{I}}} \end{pmatrix} \begin{pmatrix} \vec{\boldsymbol{c}} \\ \tilde{\vec{\boldsymbol{c}}} \end{pmatrix} = \boldsymbol{\lambda} \begin{pmatrix} \underline{\underline{\boldsymbol{B}}} & \underline{\underline{\boldsymbol{I}}} \\ \underline{\underline{\boldsymbol{I}}} & \underline{\underline{\boldsymbol{0}}} \end{pmatrix} \begin{pmatrix} \vec{\boldsymbol{c}} \\ \tilde{\vec{\boldsymbol{c}}} \end{pmatrix}} \quad . \tag{2.134}$$

This is a generalized ***symmetric eigenvalue problem*** that we are able to solve numerically after basis set truncation, which will limit the Legendre basis to only include its first $N \in \mathbb{N}$ functions. Therefore,

$$\begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix}, \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \in \mathbb{C}^{2N,2N} \quad ; \quad \begin{pmatrix} \vec{c} \\ \tilde{\vec{c}} \end{pmatrix} \in \mathbb{C}^{2N} \quad . \tag{2.135}$$

2.3.3 Numerical Calculation of $\boldsymbol{K}$, $\boldsymbol{E}$, $\boldsymbol{\psi}$

We shall now find a numerical solution to the eigenvalue problem (2.112)-(2.114). We will be again using the toy potential (1.73), calculating in arbitrary units and setting (2.39). The eigenvalue problem (2.134) was solved using the Eigen [16] package for C++ using the values $N = 127$ and $a = 25$.

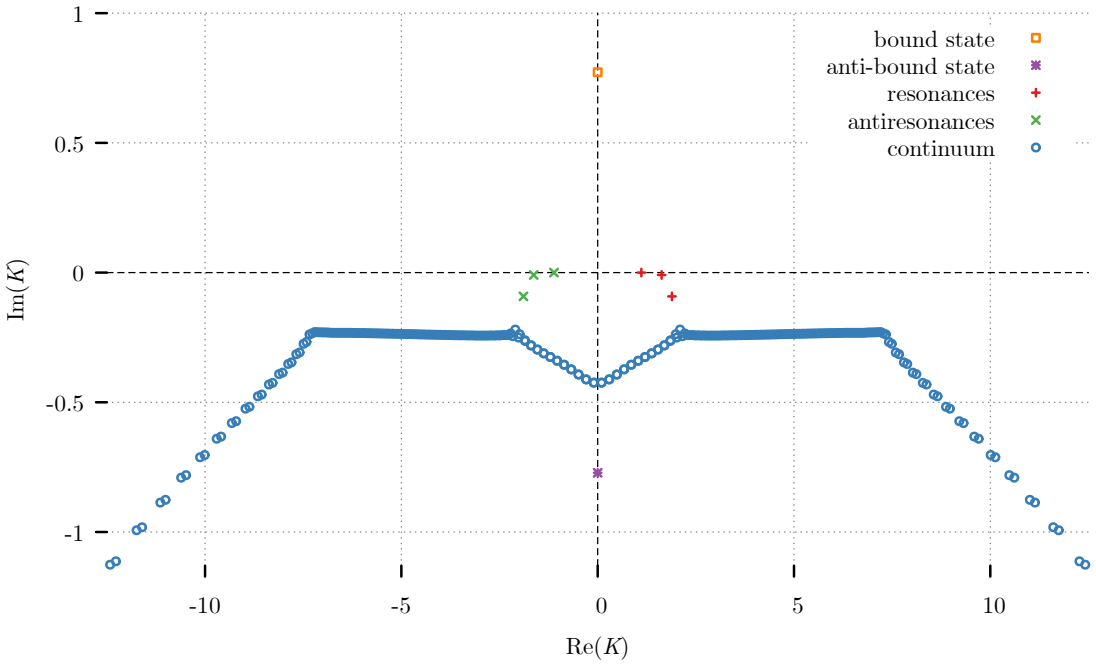

Figure 2.10: Resulting values of the wavenumber K. We see a single bound state with a real positive value of K being closely mirrored by an anti-bound state with real negative value of K. The rest of the plot is made up of resonances, anti resonances and a continuum made discrete by basis set truncation.

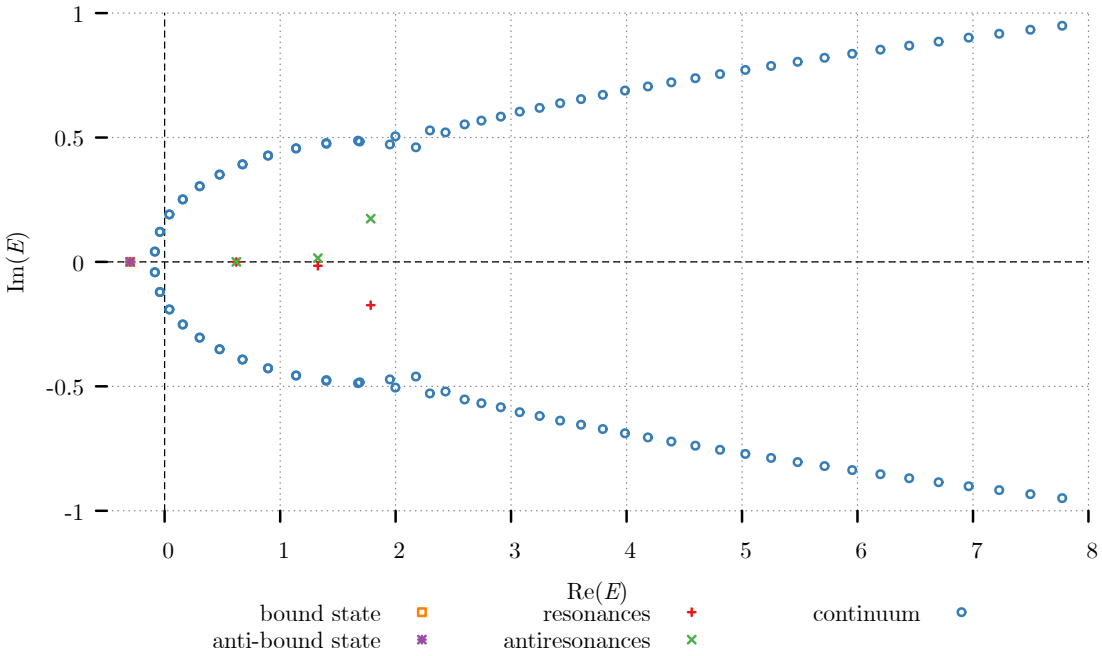

Figure 2.11: Resulting eigenvalues of $\hat{H}$. We see a single real negative energy corresponding to the bound state. The anti-bound state seen in Figure 2.10 has an energy nearly overlapping with the bound state. The rest of the plot is made up of resonances and a continuum made discrete by basis set truncation.

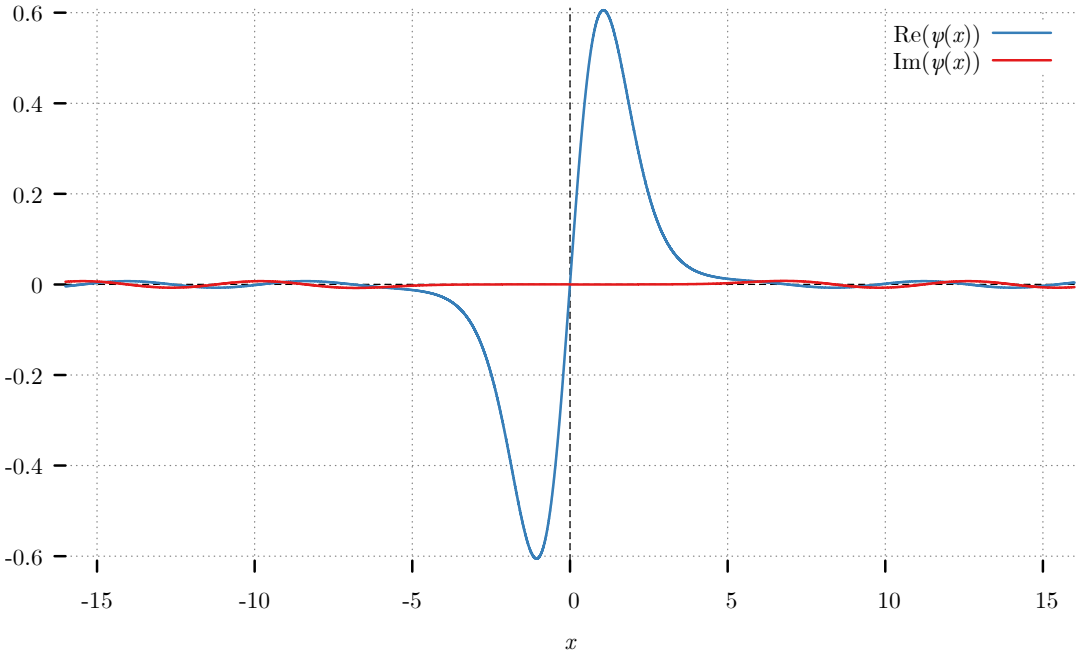

Figure 2.12: Real and imaginary parts of the first resonance wavefunction corresponding to the energy $E = 0.62097 - 5.82666 \cdot 10^{-5}i$. For small values of $|x|$ it resembles the wavefunction plotted in Figure 1.7, it however diverges for $x \to \pm\infty$, thanks to the boundary conditions (2.113)-(2.114) (though too slowly for us to be able to conveniently show it in a plot).

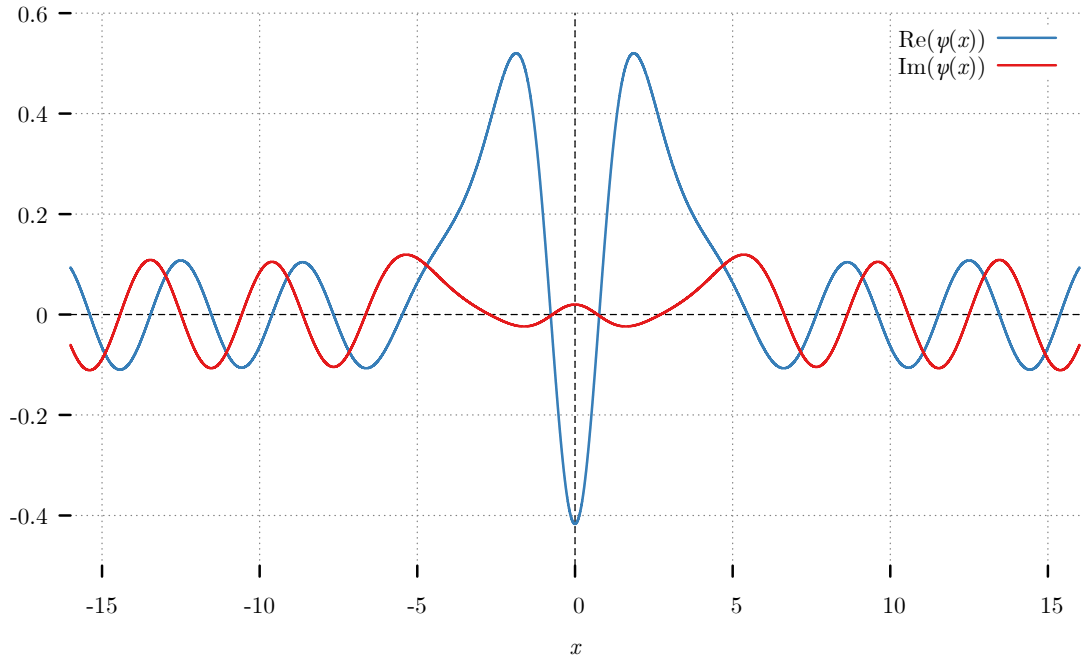

Figure 2.13: Real and imaginary parts of the second resonance wavefunction corresponding to the energy $E = 1.32720 - 0.01545i$. For small values of $|x|$ it resembles the wavefunction plotted in Figure 1.8, but it again diverges for $x \to \pm\infty$, thanks to the boundary conditions (2.113)-(2.114).

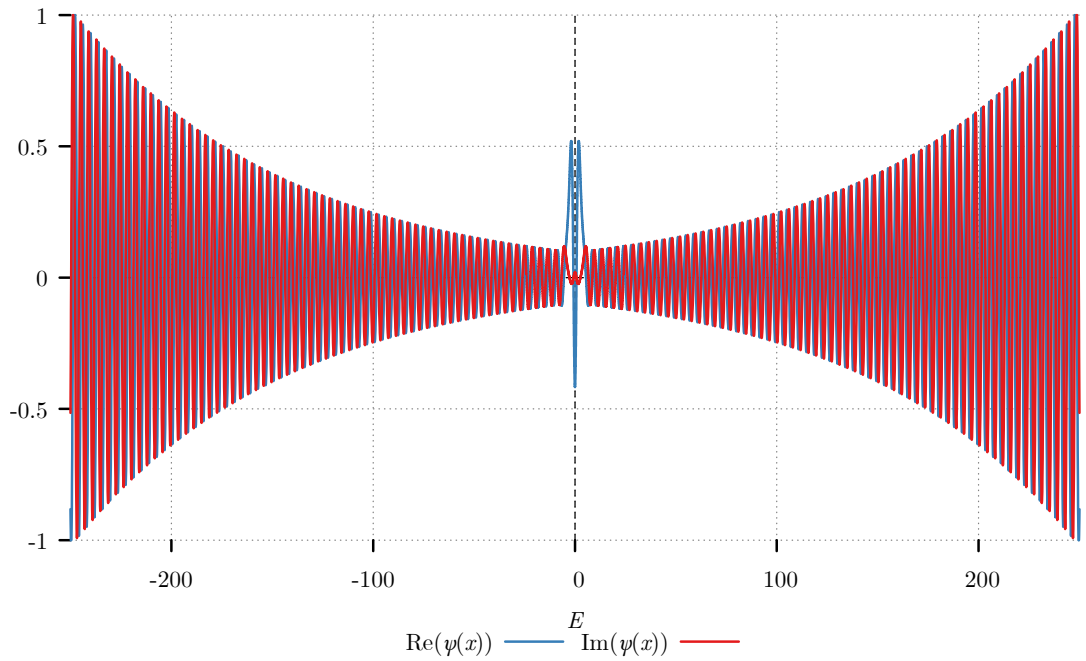

Figure 2.14: A zoomed out view of the real and imaginary parts of the second resonance wavefunction corresponding to the energy $E = 1.32720 - 0.01545i$, showing that it indeed diverges.

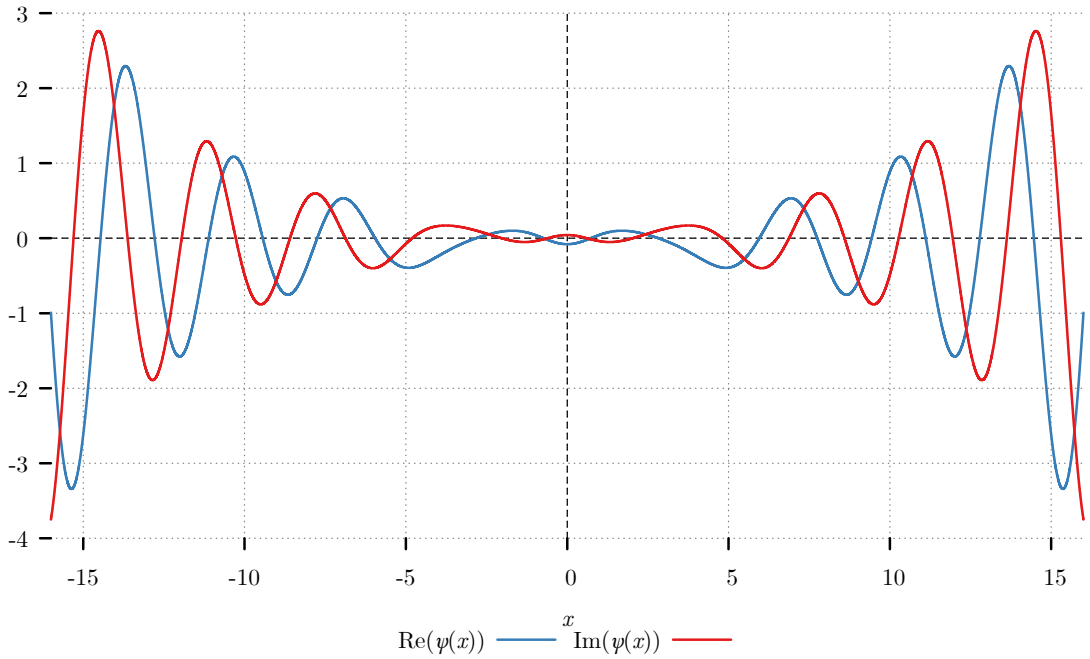

Figure 2.15: Real and imaginary parts of the third resonance wavefunction corresponding to the energy $E = 1.78458 - 0.17375i$. It also diverges for $x \to \pm\infty$, thanks to the boundary conditions (2.113)-(2.114).

2.3.4 Scalar Product, Orthonormality and Closure

Our main goal in this subsection will be to find a suitable scalar product in respect to which the just constructed Siegert states will be orthonormal and to construct a suitable closure type property. We are working with $2N$ different eigenstates (resonances, anti-resonances, bound states, anti-bound states and discretized continuum states, which arise due to the finite basis set representation of the problem). We will be distinguishing the values of $\lambda, \vec{c}, K$ and E for different eigenstates of $\hat{H}$ by superscript.

Let us now write Equation (2.134) for two different eigenvalues, $\lambda^{(n)}, \lambda^{(n')}$, and perform the following operations:

$$\begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = \lambda^{(n)} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \quad \Big| \left(\vec{c}^{\mathsf{T}(n')} \quad \tilde{\vec{c}}^{\mathsf{T}(n')} \right) \cdot \quad ;$$

$$\begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n')} \\ \tilde{\vec{c}}^{(n')} \end{pmatrix} = \lambda^{(n')} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n')} \\ \tilde{\vec{c}}^{(n')} \end{pmatrix} \quad \Big| \left(\vec{c}^{\mathsf{T}(n)} \quad \tilde{\vec{c}}^{\mathsf{T}(n)} \right) \cdot$$

$$\left(\vec{c}^{\mathsf{T}(n')} \quad \tilde{\vec{c}}^{\mathsf{T}(n')} \right) \begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = \lambda^{(n)} \left(\vec{c}^{\mathsf{T}(n')} \quad \tilde{\vec{c}}^{\mathsf{T}(n')} \right) \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \quad ;$$

$$\left(\vec{c}^{\mathsf{T}(n)} \quad \tilde{\vec{c}}^{\mathsf{T}(n)} \right) \begin{pmatrix} -\underline{\underline{A}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n')} \\ \tilde{\vec{c}}^{(n')} \end{pmatrix} = \lambda^{(n')} \left(\vec{c}^{\mathsf{T}(n)} \quad \tilde{\vec{c}}^{\mathsf{T}(n)} \right) \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n')} \\ \tilde{\vec{c}}^{(n')} \end{pmatrix} \quad .$$

Using the the fact that both matrices are symmetrical, subtracting the second equation from the first gives us

$$(\lambda^{(n)} - \lambda^{(n')}) \begin{pmatrix} \vec{c}^{\mathsf{T}(n')} & \tilde{\vec{c}}^{\mathsf{T}(n')} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = 0 \quad . \tag{2.136}$$

For $n \neq n'$, $\lambda^{(n)} \neq \lambda^{(n')}$; therefore,

$$\begin{pmatrix} \vec{c}^{\mathsf{T}(n')} & \tilde{\vec{c}}^{\mathsf{T}(n')} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = 0 \quad . \tag{2.137}$$

Theorem 3. *Let $n \in \{1, 2, \ldots, 2N\}$. Then*

$$\begin{pmatrix} \vec{c}^{\mathsf{T}(n)} & \tilde{\vec{c}}^{\mathsf{T}(n)} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \neq 0 \quad . \tag{2.138}$$

Proof. We will prove the statement by contradiction. Let us assume that

$$\begin{pmatrix} \vec{c}^{\mathsf{T}(n'} & \tilde{\vec{c}}^{\mathsf{T}(n')} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = 0 \quad .$$

This means that vector

$$\begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix}$$

is perpendicular to every vector in $\mathbb{C}^{2N}$, and therefore

$$\begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = 0 \quad .$$

By applying the same argument again we can see that

$$\begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = 0 \quad .$$

But this contradicts the fact that $\begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix}$ is an eigenvector. □

Using (2.137)-(2.138), we see that the relation

$$\begin{pmatrix} \vec{c}^{\mathsf{T}(n')} & \tilde{\vec{c}}^{\mathsf{T}(n')} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \tag{2.139}$$

is a good candidate for a scalar product of vectors $\vec{c}^{(n)}$ and $\vec{c}^{(n')}$. And that in respect to this scalar product vectors $\vec{c}^{(n)}$ will be orthogonal.

Orthonormality relations. *Let $n, n' \in \{1, 2, \ldots, 2N\}$. We conveniently introduce a normalization convention such that*

$$\begin{pmatrix} \vec{c}^{\mathsf{T}(n')} & \tilde{\vec{c}}^{\mathsf{T}(n')} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = \delta_{nn'} 2\lambda^{(n)} \quad . \tag{2.140}$$

Adding the factor $2\lambda^{(n)}$ is a useful convention that will simplify certain expressions in the future.

Closure.

$$\sum_{n=1}^{2N} \frac{1}{2\lambda^{(n)}} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \begin{pmatrix} \vec{c}^{\mathsf{T}(n)} & \tilde{\vec{c}}^{\mathsf{T}(n)} \end{pmatrix} = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{I}} \\ \underline{\underline{I}} & -\underline{\underline{B}} \end{pmatrix} \quad . \tag{2.141}$$

Proof. Let $\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} \in \mathbb{C}^{2N}$. Then $\exists q_1, q_2, \ldots, q_{2N} \in \mathbb{C}$ such that

$$\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} = \sum_{n=1}^{2N} q_n \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix}$$

$$\forall n \in \{1, 2, \ldots, 2N\}, \quad q_n = \frac{1}{2\lambda^{(n)}} \begin{pmatrix} \vec{u}^{\mathsf{T}} & \vec{v}^{\mathsf{T}} \end{pmatrix} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix}$$

Let us now define the matrix

$$\underline{\underline{Q}} \coloneqq \sum_{n=1}^{2N} \frac{1}{2\lambda^{(n)}} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \begin{pmatrix} \vec{c}^{\mathsf{T}(n)} & \tilde{\vec{c}}^{\mathsf{T}(n)} \end{pmatrix} \in \mathbb{C}^{2N \times 2N} \quad . \tag{2.142}$$

We see that

$$\begin{aligned} &\underline{\underline{Q}} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} = \\ &= \sum_{n=1}^{2N} \frac{1}{2\lambda^{(n)}} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \begin{pmatrix} \vec{c}^{\mathsf{T}(n)} & \tilde{\vec{c}}^{\mathsf{T}(n)} \end{pmatrix} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} \sum_{n'=1}^{2N} q_{n'} \begin{pmatrix} \vec{c}^{(n')} \\ \tilde{\vec{c}}^{(n')} \end{pmatrix} = \\ &= \sum_{n=1}^{2N} \frac{1}{2\lambda^{(n)}} \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} \sum_{n''=1}^{2N} q_{n'} 2\lambda^{(n)} \delta_{nn'} = \sum_{n=1}^{2N} q_n \begin{pmatrix} \vec{c}^{(n)} \\ \tilde{\vec{c}}^{(n)} \end{pmatrix} = \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} \quad . \end{aligned} \tag{2.143}$$

Therefore, $\underline{\underline{Q}} \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix}$ is the $2N \times 2N$ unit matrix. This means that

$$\underline{\underline{Q}} = \begin{pmatrix} \underline{\underline{B}} & \underline{\underline{I}} \\ \underline{\underline{I}} & \underline{\underline{0}} \end{pmatrix}^{-1} = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{I}} \\ \underline{\underline{I}} & -\underline{\underline{B}} \end{pmatrix} \quad . \tag{2.144}$$

□

This is an unconventional closure type property, different to the one encountered in HQM. It can sometimes be useful to rewrite the closure relations as the system of equations

$$\sum_{n=1}^{2N} \vec{c}^{(n)} \vec{c}^{\intercal(n)} = 2\underline{\underline{I}} \quad ;$$
$$\sum_{n=1}^{2N} \frac{1}{\lambda^{(n)}} \vec{c}^{(n)} \vec{c}^{\intercal(n)} = \underline{\underline{0}} \quad ;$$
$$\sum_{n=1}^{2N} \lambda^{(n)} \vec{c}^{(n)} \tilde{\vec{c}}^{\intercal(n)} = -2\underline{\underline{B}} \quad .$$

2.3.5 Siegert Pseudostate Representation of the Retarded Propagator

In this subsection we will discuss nonhermitian Siegert based ways of calculating the so-called retarded Green function and the transmission coefficient, previously encountered in Chapter 1 and later on Chapter 2 in Subsection 2.2. We will be working with the retarded Green operator

$$\hat{G}^{+}(E) = \frac{1}{E - \hat{H} + i\epsilon} \quad ; \quad E \in \mathbb{R} \quad ; \tag{2.145}$$

seen in Chapter 1, in (1.35), and with its position representation

$$G_E^{+}(x, y) = \langle x | \, \hat{G}^{+}(E) \, | y \rangle \quad ; \tag{2.146}$$

known as the retarded Green function.

Our above constructed Siegert pseudostates are expanded in the used basis set as detailed in Equation (2.122). That is,

$$\psi^{(n)}(x) = \sum_{\nu=1}^{N} c_{\nu}^{(n)} b_{\nu}(x) \quad . \tag{2.147}$$

It can be shown that the retarded Green function (2.146) can be calculated using the functions $\psi^{(n)}(x)$ as [38], [42]

$$\boldsymbol{G_E^{+}(x, y) = \frac{m}{\hbar^2} \sum_{n=1}^{2N} \frac{\psi^{(n)}(x)\psi^{(n)}(y)}{K^{(n)}(K - K^{(n)})}} \quad ; \tag{2.148}$$

where again

$$K^{(n)} = -i\lambda^{(n)}, \quad \hbar K^{(n)} = \sqrt{2mE^{(n)}} \quad . \tag{2.149}$$

The retarded Green function $G_E^{+}(x, y)$ appears ubiquitously in the conventional quantum mechanics and ***contains all the information about scattering phenomena***. Yet Equation (2.148) managed to express $G_E^{+}(x, y)$ in an equivalent nonhermitian fashion in terms of the Siegert pseudostates. The operator $\hat{G}^{+}(E)$ is

the so-called propagator, and it can be obtained as a Fourier transformation of the time evolution operator $\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$ [42]

$$\int_0^\infty \mathrm{d}t\, \hat{U}(t) e^{\frac{i}{\hbar}\hat{E}t} = \int_0^\infty \mathrm{d}t\, e^{\frac{i}{\hbar}(E-\hat{H}+i\epsilon)t} = \frac{e^{\frac{i}{\hbar}(E-\hat{H}+i\epsilon)t}}{\frac{i}{\hbar}(E-\hat{H}+i\epsilon)t}\Big|_0^\infty = i\hbar\hat{G}^+(E) \quad . \quad (2.150)$$

It can also be shown that the transmission coefficient, which we have already encountered and calculated in Chapter 1, using methods of HQM, as well as earlier in this chapter in Subsection 2.2.11, using complex scaling, can be calculated as [38], [42]

$$\boxed{T_E^+ = ike^{-2ika} \sum_{n=1}^{2N} \frac{\psi^{(n)}(-a)\psi^{(n)}(a)}{K^{(n)}(K-K^{(n)})}} \quad . \quad (2.151)$$

Here T_E^+ is expressed as a sum over separate contributions arising from all kinds of the Siegert pseudostates.

2.3.6 Numerical Calculation of T_E^+

We will now use the formula (2.151) with the values of $K^{(n)}$ and $\psi^{(n)}(x)$ calculated in Subsection 2.3.3 to determine the value of T_E^+.

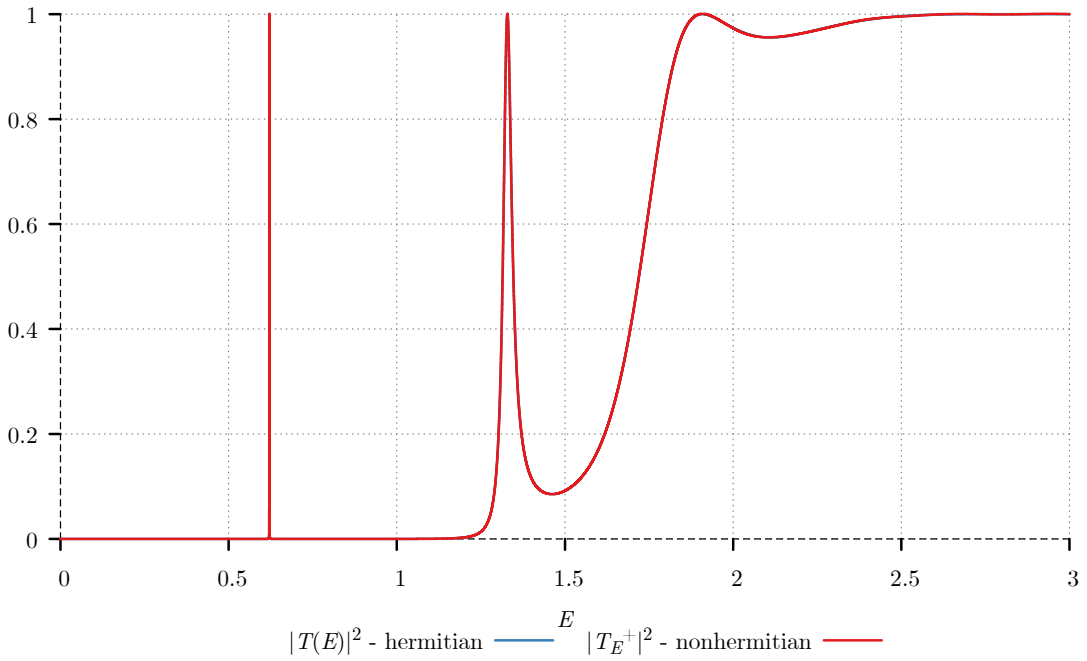

Figure 2.16: The resulting transmission probability, calculated using the formula (2.151), overlaid with the hermitian calculation of the transmission probability made in Chapter 1, plotted in Figure 1.2. We see that their values closely match. Small discrepancies are caused by the basis set truncation an other approximation used.

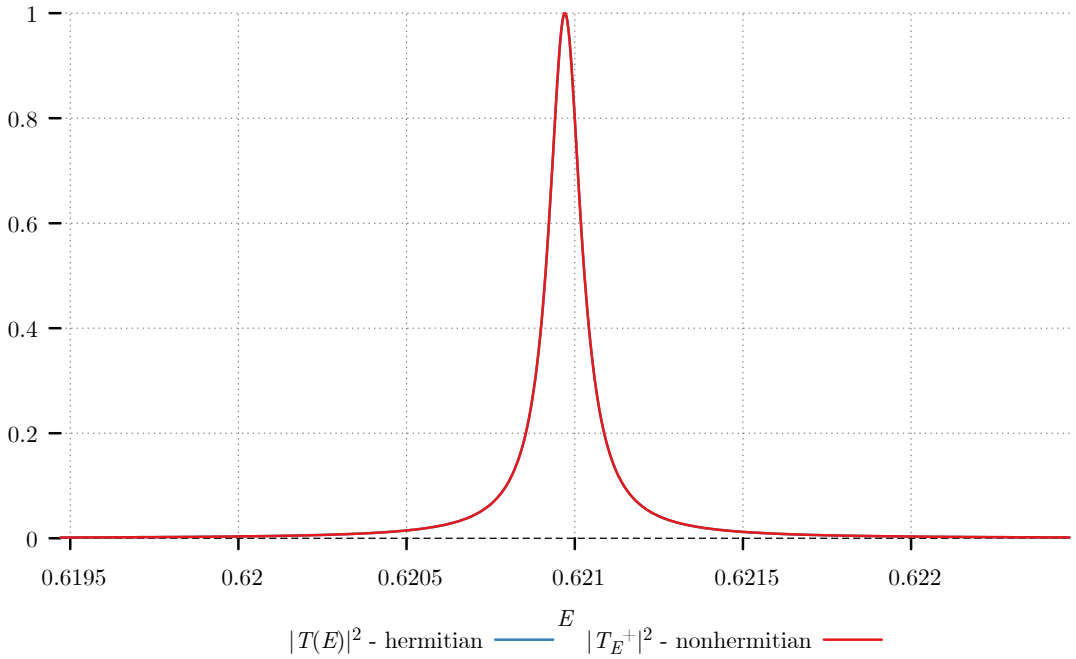

Figure 2.17: The squared norm of the first addend in the sum (2.151), representing the contribution of the first resonance to the transmission probability overlaid with the first peak in transmission probability, calculated in Chapter 1, corresponding to the first resonance, plotted in Figure 1.3. We see that their values very closely match.

2.3.7 Summary

In this section we have described the method of ***Siegert pseudostates*** and illustrated its applicability on our simple toy model. We have obtained explicitly the relevant Siegert eigensolutions (associated with the bound, anti-bound, resonance, and anti-resonance states), as well as their corresponding wavefunctions. Appropriate orthonormality and closure relations for the Siegert pseudostates have been established, and the Siegert based scattering theory has been formulated.

The main advantage of this approach is that we can calculate all kinds of Siegert states (bound, anti-bound, resonance, and anti-resonance states), not just bound states and resonances as we did in the case of complex scaling. Moreover, the Siegert pseudostate scattering theory leads towards extremely simple and elegant formulas for the ***retarded propagator*** $\hat{G}^+(E)$, for the ***transmission coefficient*** $\hat{T}_E^+$ and for other quantities. Also the time propagation of hermitian wavepackets can be conveniently performed using the Siegert pseudostates as a basis.

The main disadvantage of this method lies so far in its limited applicability. (It has not been formulated so far for general multidimensional and multichannel problems.) But the formalism is still an active field of research and these problems could thus be solved in the future.

2.4 Anti-bound States and their Mathematical and Physical Meaning

Physical meaning of bound states is evident from any introductory quantum mechanical textbook. Physical meaning of (anti-)resonances has been clarified enough in this thesis (see in particular Breit-Wigner peaks in the $|T(E)|^2$), both using complex scaling (see Section 2.2) and the Siegert pseudostate formalism (see Section 2.3). On the other hand, physical meaning of the anti-bound (virtual) states, or even their mathematical significance, remains much less clear. The literature dealing with anti-bound states is rather scarce, and it is quite possible that additional and important insights regarding anti-bound states will emerge from the still ongoing research. Some valuable insights have nevertheless been found. Let us now briefly mention some existing and insightful works dealing with the anti-bound states:

- Zavin et al. [45] examine the role which an anti-bound state plays when a bound state penetrates into continuum (via reducing continuously the depth of a rectangular potential well).
- Klaiman et al. [22] discuss anti-bound states in the context of absolute position of a resonance peak (resonances below the threshold).
- The phenomenon of bound state entering a continuum has been investigated further by Garmon [14] who related this penetration of a bound state into a continuum to an amplification of non-Markovian decay.
- Vertse et al. [5], [25], [44] have examined anti-bound states for 1D model potentials relevant to nuclear physics.
- Anti-bound states in the context of nuclear physics are also being studied by Uzikov [43].
- A group theoretical study involving anti-bound states has been performed by Guerrero [17].
- Inner products involving anti-bound states have been investigated in a mathematical study of Julve [20].
- Anti-bound states for a 2-by-2 coupled channel problem have been studied by Abdelmoula [1].
- Additional works include, e.g. the papers of Tanimu [40] who studied anti bound states in double and triple potential wells.
- Last but not least, anti-bound states proved to play an important role in electron-molecule scattering, see the papers of Čížek and Houfek [11], [12], Čurík [18], Mašín [28] and references therein.

Chapter 3

Interaction of Atoms with Laser

3.1 Introduction

In this chapter we will overview the problem of interaction of an atom with a laser pulse. We will introduce powerful formalism of ***Floquet theory***, and show subsequently how laser induced resonances arise in atomic systems. An emergence of resonances naturally leads us towards invoking the language of NHQM in the present context of laser driven atoms. Most importantly, our nonhermitian analysis of the problem will ultimately result in formation of a nonhermitian degeneracy known as an ***exceptional point*** (EP). We will then numerically calculate the corresponding parameters of the laser pulse, which will result in a creation of such an EP. Peculiar non-intuitive properties of an EP will then be discussed.

3.2 Basic Framework

Let us motivate our considerations by recalling the textbook problem of a Hydrogen atom in an external electromagnetic field [19]. The Hamiltonian for a free hydrogen atom is

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} + V(\hat{\vec{x}}) = -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \quad ; \quad V(\vec{x}) = -\frac{Ze^2}{|\vec{x}|} \quad ; \tag{3.1}$$

where m is the mass of an electron, $\vec{x}$ the position of the electron relative to the nucleus and Ze the charge of the nucleus.

The incoming electromagnetic field can be described by its vector potential, $\vec{A}(t, \vec{y})$, with the Coulomb gauge

$$\vec{\nabla} \cdot \vec{A}(t, \vec{y}) = 0 \quad . \tag{3.2}$$

The transverse electric and magnetic fields in Gaussian units can be expressed in terms of the vector potential $\vec{A}(t, \vec{y})$ as [19]

$$\vec{E}(t, \vec{y}) = -\frac{1}{c}\partial_t \vec{A}(t, \vec{y}) \quad ; \tag{3.3}$$

$$\vec{B}(t, \vec{y}) = \vec{\nabla} \times \vec{A}(t, \vec{y}) \quad . \tag{3.4}$$

For the sake of simplicity, we consider here only a classical electromagnetic field (not quantized).

Let us recall now the nature of coupling between the Hydrogen atom and the electromagnetic field. To further simplify the following calculations, and consistently with a well established practice, we neglect the electromagnetic field created due to electron acceleration. Then $\vec{A}(t, \vec{y})$ is not modified by the presence of an atom, and corresponds to the vector potential of a free laser pulse. The adequate Hamiltonian of the Hydrogen atom exposed to an external laser field then takes the following appearance [19]:

$$\hat{H}_{\mathrm{MG}}(t) \coloneqq \frac{1}{2m}\left(\hat{\vec{p}} - \frac{q}{c}\vec{A}(t, \vec{x})\right)^2 + V(\hat{\vec{x}}) \quad . \tag{3.5}$$

This is the well known momentum gauge (minimum coupling) form of the Hamiltonian. The formula (3.11) is obtained from (3.1) via the formal replacement

$$\hat{\vec{p}} \mapsto \hat{\vec{p}} - \frac{q}{c}\vec{A}(t, \vec{x}) \quad . \tag{3.6}$$

For our subsequent purposes, and in accordance with a common practice when dealing with matter-laser interaction, we will now conveniently impose two simplifications. First, we will adopt the dipole approximation

$$\vec{A}(t, \vec{x}) = \vec{A}(t) \quad ; \tag{3.7}$$

while assuming tacitly that the wavelength of the used laser is much larger than spatial dimensions of the atomic system. (This assumption is well justified in the infrared, optical, and ultraviolet range of the spectrum.) Second, we will reduce the number of spatial dimensions from three to one. In other words, instead of a 3D Hydrogen atom, we will study from now a 1D model problem characterized by the momentum gauge Hamiltonian

$$\hat{H}_{\mathrm{MG}}(t) = \frac{1}{2m}\left(\hat{p} - \frac{q}{c}A(t)\right)^2 + V(\hat{x}) \quad ; \tag{3.8}$$

where $V(x)$ is again the familiar toy potential (1.73) (not the Coulomb potential). In this model the electric field (3.3) takes on the following form:

$$E(t) = -\frac{1}{c}\partial_t A(t) \quad . \tag{3.9}$$

Quantum dynamics of our 1D model atom driven by laser is governed by the usual time dependent Schrödinger equation (TDSE)

$$i\hbar\partial_t \left|\psi(t)\right\rangle = \hat{H}_{\mathrm{MG}}(t) \left|\psi(t)\right\rangle \quad . \tag{3.10}$$

Further theoretical analysis of Equation (3.10) is facilitated by means of unitary (gauge) transformations, which provide useful alternative representations of the atom-laser interaction, and which bring additional physics insights.

3.3 Gauge Transformations

3.3.1 Momentum Gauge

After multiplying out the squared term in (3.5), the momentum gauge Hamiltonian takes on the appearance

$$\hat{\boldsymbol{H}}_{\mathrm{MG}}(\boldsymbol{t}) = \frac{\hat{\boldsymbol{p}}^2}{\boldsymbol{2m}} + \boldsymbol{V}(\hat{\boldsymbol{x}}) - \frac{\boldsymbol{q}}{\boldsymbol{mc}}\boldsymbol{A}(\boldsymbol{t})\hat{\boldsymbol{p}} + \frac{\boldsymbol{q}^2}{\boldsymbol{2mc^2}}\boldsymbol{A}^2(\boldsymbol{t}) \quad . \tag{3.11}$$

We see that the first two terms of (3.11) make up the standard atomic Hamiltonian without the presence of a laser. The remaining two terms thus account for the influence of the laser.

We denote the state vectors corresponding to $\hat{H}_{\mathrm{MG}}(t)$ in time t as $|\psi_{\mathrm{MG}}(t)\rangle$. The corresponding TDSE then reads as follows:

$$i\hbar\partial_t |\psi_{\mathrm{MG}}(t)\rangle = \hat{H}_{\mathrm{MG}}(t) |\psi_{\mathrm{MG}}(t)\rangle \quad . \tag{3.12}$$

3.3.2 Reduced Momentum Gauge

We shall now derive the so-called reduced momentum gauge Hamiltonian. This will be an intermediate preparatory step to deriving subsequently the length and acceleration gauges. Let us now define the reduced momentum gauge state vector at time t by the following relation:

$$|\psi_{\mathrm{MG}}(t)\rangle =: e^{if_1(t)} |\psi_{\mathrm{RMG}}(t)\rangle \quad ; \tag{3.13}$$

where $f_1(t)$ is a yet to be determined function of time.

By substituting (3.13) into (3.12) we get

$$\begin{aligned} &i\hbar e^{if_1(t)}\partial_t |\psi_{\mathrm{RMG}}(t)\rangle - \hbar f_1'(t) e^{if_1(t)} |\psi_{\mathrm{RMG}}(t)\rangle = \\ &= \left(\frac{\hat{p}^2}{2m} - \frac{q}{mc}A(t)\hat{p} + \frac{q^2}{2mc^2}A^2(t) + V(\hat{x})\right) e^{if_1(t)} |\psi_{\mathrm{RMG}}(t)\rangle \end{aligned} \tag{3.14}$$

$$\begin{aligned} &i\hbar\partial_t |\psi_{\mathrm{RMG}}(t)\rangle = \\ &= \left(\frac{\hat{p}^2}{2m} - \frac{q}{mc}A(t)\hat{p} + V(\hat{x})\right) |\psi_{\mathrm{RMG}}(t)\rangle + \left(\frac{q^2}{2mc^2}A^2(t) + \hbar f_1'(t)\right) |\psi_{\mathrm{RMG}}(t)\rangle \quad . \end{aligned} \tag{3.15}$$

We aim to simplify this equation by choosing $f_1(t)$ in such a way that the last r.h.s. term cancels out. This happens when

$$-\hbar f_1'(t) = \frac{q^2}{2mc^2}A^2(t) \tag{3.16}$$

$$f_1(t) = -\frac{1}{\hbar}\frac{q^2}{2mc^2}\int_{t_0}^{t} A^2(t')\,\mathrm{d}t' \quad . \tag{3.17}$$

Therefore,

$$i\hbar\partial_t |\psi_{\mathrm{RMG}}(t)\rangle = \hat{H}_{\mathrm{RMG}}(t) |\psi_{\mathrm{RMG}}(t)\rangle \quad ; \tag{3.18}$$

where

$$\hat{\boldsymbol{H}}_{\mathrm{RMG}}(t) \coloneqq \frac{\hat{\boldsymbol{p}}^2}{2\boldsymbol{m}} + \boldsymbol{V}(\hat{\boldsymbol{x}}) - \frac{\boldsymbol{q}}{\boldsymbol{mc}}\boldsymbol{A}(\boldsymbol{t})\hat{\boldsymbol{p}} \tag{3.19}$$

is called the reduced momentum gauge Hamiltonian. This is because the interaction with the laser is facilitated by the momentum operator $\hat{p}$, via the term $-\frac{q}{mc}A(t)\hat{p}$.

3.3.3 Length Gauge

Let us now define the length gauge state vector in time t by the following relation:

$$|\psi_{\mathrm{RMG}}(t)\rangle =: e^{if_2(t)\hat{x}} |\psi_{\mathrm{LG}}(t)\rangle \quad ; \tag{3.20}$$

where $f_2(t)$ is a yet to be determined function of time. By substituting (3.19) and (3.20) into (3.18) we get

$$\begin{aligned}
&i\hbar e^{if_2(t)\hat{x}}\partial_t |\psi_{\mathrm{LG}}(t)\rangle - \hbar f_2'(t) e^{if_2(t)\hat{x}} x |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) - \frac{q}{mc}A(t)\hat{p}\right) e^{if_2(t)\hat{x}} |\psi_{\mathrm{LG}}(t)\rangle \quad \Big| e^{-if_2(t)\hat{x}}\boldsymbol{.} \qquad (3.21)\\
&i\hbar\partial_t |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{1}{2m} e^{-if_2(t)\hat{x}}\hat{p}^2 e^{if_2(t)\hat{x}} + V(\hat{x}) + \hbar f_2'(t)\hat{x} - \frac{q}{mc}A(t) e^{-if_2(t)\hat{x}}\hat{p}e^{if_2(t)\hat{x}}\right) |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{1}{2m}\left(\hat{p}^2 - if_2(t)[\hat{x},\hat{p}^2] - \frac{1}{2}f_2^2(t)[\hat{x},[\hat{x},\hat{p}^2]]\right) + V(\hat{x}) + \hbar f_2'(t)\hat{x} + \right. \\
&\left. -\frac{q}{mc}A(t)\left(\hat{p} - if_2(t)[\hat{x},\hat{p}]\right)\right) |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{1}{2m}\left(\hat{p}^2 + 2i\hbar f_2(t) - i\hbar f_2^2(t)[\hat{x},\hat{p}^2]\right) + V(\hat{x}) + \hbar f_2'(t)\hat{x} + \right. \\
&\left. -\frac{q}{mc}A(t)\left(\hat{p} + \hbar f_2(t)\right)\right) |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + \frac{1}{m}\left(\hbar f_2(t) - \frac{q}{c}A(t)\right)\hat{p} + V(\hat{x}) + \hbar f_2'(t)\hat{x} + \right. \\
&\left. +\frac{\hbar}{m}f_2(t)\left(\hbar f_2(t) - \frac{q}{c}A(t)\right)\right) |\psi_{\mathrm{LG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) + \hbar f_2'(t)\hat{x}\right) |\psi_{\mathrm{LG}}(t)\rangle + \frac{1}{m}\left(\hbar f_2(t) - \frac{q}{c}A(t)\right)\left(\hat{p} + \hbar f_2(t)\right) |\psi_{\mathrm{LG}}(t)\rangle \quad . \qquad (3.22)
\end{aligned}$$

Where we used the Baker–Campbell–Hausdorff relationship [33]. We are again trying to cancel out the last term of the equation, giving us

$$f_2(t) = -\frac{q}{\hbar c}A(t) \quad . \tag{3.23}$$

Therefore,

$$i\hbar\partial_t |\psi_{\mathrm{LG}}(t)\rangle = \hat{H}_{\mathrm{LG}}(t) |\psi_{\mathrm{LG}}(t)\rangle \quad ; \tag{3.24}$$

where

$$\hat{\boldsymbol{H}}_{\mathrm{LG}} = \frac{\hat{\boldsymbol{p}}^2}{2\boldsymbol{m}} + \boldsymbol{V}(\hat{\boldsymbol{x}}) + \boldsymbol{qE}(\boldsymbol{t})\hat{\boldsymbol{x}} \quad ; \quad E(t) = -\frac{1}{c}\partial_t A(t) \tag{3.25}$$

is the length momentum gauge Hamiltonian. We see that again the first two terms of the equation make up the standard atomic Hamiltonian without the presence of a laser. The remaining term thus accounts for the influence of the laser, which in this case happens through the position operator $\hat{x}$, that is why we call this the length gauge. Notice that the last term of (3.25), $qE(t)\hat{x}$, is the energy of the dipole $q\hat{x}$ in an external electric field $E(t)$.

3.3.4 Acceleration Gauge

We will define the acceleration gauge state vector in time t by the following relation:

$$|\psi_{\mathrm{RMG}}(t)\rangle =: e^{if_3(t)\hat{p}}\,|\psi_{\mathrm{AG}}(t)\rangle \quad ; \tag{3.26}$$

where $f_3(t)$ is a yet to be determined function of time. By substituting (3.19) and (3.26) into (3.18) we get

$$\begin{aligned}
&i\hbar e^{if_3(t)\hat{p}}\partial_t\,|\psi_{\mathrm{AG}}(t)\rangle - \hbar f_3'(t)e^{if_3(t)\hat{p}}\hat{p}\,|\psi_{\mathrm{AG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) - \frac{q}{mc}A(t)\hat{p}\right) e^{if_3(t)\hat{p}}\,|\psi_{\mathrm{AG}}(t)\rangle \quad \Big| e^{-if_3(t)\hat{p}}\cdot \qquad (3.27)\\
&i\hbar\partial_t\,|\psi_{\mathrm{AG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + e^{-if_3(t)\hat{p}}V(\hat{x})e^{if_3(t)\hat{p}} + \hbar f_3'(t)\hat{p} - \frac{q}{mc}A(t)\hat{p}\right)|\psi_{\mathrm{AG}}(t)\rangle = \\
&= \left(\frac{\hat{p}^2}{2m} + V(\hat{x}+\hbar f_3(t))\right)|\psi_{\mathrm{AG}}(t)\rangle + \left(\hbar f_3'(t) - \frac{q}{mc}A(t)\right)\hat{p}\,|\psi_{\mathrm{AG}}(t)\rangle \quad ; \qquad (3.28)
\end{aligned}$$

where we used the fact that the translation operator $e^{\frac{i}{\hbar}\hat{p}\xi}$ satisfies the relation

$$\forall g \in \mathrm{C}(\mathbb{R},\mathbb{C}) \quad ; \quad \forall x,\xi \in \mathbb{R} \quad ; \quad e^{-\frac{i}{\hbar}\hat{p}\xi}g(x)e^{\frac{i}{\hbar}\hat{p}\xi} = g(x+\xi) \quad . \tag{3.29}$$

Again, in order for the last term to cancel out, we set

$$\hbar f_3'(t) = \frac{q}{mc}A(t) \tag{3.30}$$

$$f_3(t) = \frac{1}{\hbar}\frac{q}{mc}\int_{t_0}^{t} A(t')\,\mathrm{d}t' \quad . \tag{3.31}$$

Therefore,

$$i\hbar\partial_t\,|\psi_{\mathrm{AG}}(t)\rangle = \hat{H}_{\mathrm{AG}}(t)\,|\psi_{\mathrm{AG}}(t)\rangle \quad ; \tag{3.32}$$

where

$$\boxed{\hat{\boldsymbol{H}}_{\mathbf{AG}}(\boldsymbol{t}) = \frac{\hat{\boldsymbol{p}}^{\boldsymbol{2}}}{\boldsymbol{2m}} + \boldsymbol{V}(\hat{\boldsymbol{x}} + \boldsymbol{\alpha}(\boldsymbol{t}))} \quad ; \quad \alpha(t) = \frac{q}{mc}\int_{t_0}^{t} A(t')\,\mathrm{d}t' \tag{3.33}$$

is the acceleration gauge Hamiltonian. The effect of the laser is incorporated here into the displacement of the potential $V(\hat{x})$ by a time dependent shift term $\alpha(t)$.

Importantly, for large values of $|x|$, the potential term $V(\hat{x}+\alpha(t))$ falls off to zero, and the Hamiltonian (3.33) is thus reduced to the Hamiltonian of a free

particle, $\hat{H}_0 = \frac{\hat{p}^2}{2m}$. In other words, our quantum particle (e.g. an electron) does not feel the effect of the laser at large distances from the atom. This enables us to study laser assisted scattering of electrons on atoms by means of the scattering formalism which was described above in Chapters 1-2. Indeed, the fundamental prerequisite of scattering theory – the asymptotic condition – holds for the just presented acceleration gauge Hamiltonian of Equation (3.33). This is the basic advantage of the acceleration gauge compared to the momentum and length gauges (where the formulation of scattering theory is in principle also possible, but much more formally complicated).

Weak Field Regime

If we assume weak laser intensity (small enough values of $\alpha(t)$), we can, using Taylor expansion, make the following approximation:

$$\hat{\boldsymbol{H}}_{\mathbf{AG}}(\boldsymbol{t}) \approx \frac{\hat{\boldsymbol{p}}^{\boldsymbol{2}}}{\boldsymbol{2m}} + \boldsymbol{V}(\hat{\boldsymbol{x}}) + \boldsymbol{V'}(\hat{\boldsymbol{x}})\boldsymbol{\alpha}(\boldsymbol{t}) \quad . \tag{3.34}$$

Equation (3.34) explains neatly the name acceleration gauge: The effect of laser is incorporated in the last term, which contains $V'(\hat{x})$, i.e. the acceleration of the electron.

3.3.5 Monochromatic Laser Light

From now on we will assume that the incoming electromagnetic radiation corresponds to monochromatic laser light. This assumption is justified, since the incoming electromagnetic pulse has a slowly varying envelope, supporting many optical cycles. The vector potential then takes the following form:

$$A(t) = A_0 \sin(\omega t) \quad ; \tag{3.35}$$

where ω is the corresponding laser frequency. Therefore,

$$E(t) = -\frac{1}{c}\partial_t A(t) = -A_0 \frac{1}{c}\partial_t \sin(\omega t) = E_0 \cos(\omega t) \quad ; \tag{3.36}$$

$$\alpha(t) = \frac{q}{mc}\int_{t_0}^{t} A(t')\,\mathrm{d}t' = A_0 \frac{q}{mc}\int_{t_0}^{t} \sin(\omega t')(t')\,\mathrm{d}t' = \alpha_0 \cos(\omega t) \quad ; \tag{3.37}$$

where

$$E_0 = -A_0\frac{\omega}{c} \quad ; \quad \alpha_0 = -\frac{q}{\omega mc}A_0 \quad . \tag{3.38}$$

The coefficient α_0 is called the ***quiver amplitude***. The different gauge Hamiltonians become

$$\hat{H}_{\mathrm{MG}}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x}) - \frac{q}{mc}A_0 \sin(\omega t)\hat{p} + \frac{q^2}{2mc^2}A_0^2 \sin^2(\omega t) \quad ; \tag{3.39}$$

$$\hat{H}_{\mathrm{RMG}}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x}) - \frac{q}{mc}A_0 \sin(\omega t)\hat{p} \quad ; \tag{3.40}$$

$$\hat{H}_{\mathrm{LG}}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x}) + qE_0 \cos(\omega t)\hat{x} \quad ; \tag{3.41}$$

$$\hat{H}_{\mathrm{AG}}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x} + \alpha_0 \cos(\omega t)) \approx \frac{\hat{p}^2}{2m} + V(\hat{x}) + V'(\hat{x})\alpha_0 \cos(\omega t) \quad . \tag{3.42}$$

Since the incoming electromagnetic pulse is oscillating, it gives kicks to the electron and thus creates a possibility for its excitation and even for its detachment from the atom (ionization) [8].

3.4 Floquet Theory

3.4.1 Introduction and Motivation

We are interested to study light induced dynamics of an atom. This would imply to solve the TDSE (3.32), which for monochromatic fields takes the form

$$i\hbar\partial_t \left|\psi_{\mathrm{AG}}(t)\right\rangle = \hat{H}_{\mathrm{AG}}(t) \left|\psi_{\mathrm{AG}}(t)\right\rangle \quad ; \tag{3.43}$$

where

$$\hat{H}_{\mathrm{AG}}(t) = -\frac{\hbar^2}{2m}\partial_{xx} + V(x + \alpha_0 \cos(\omega t)) \quad ; \tag{3.44}$$

see the previous section.

Importantly, in the case of monochromatic (time periodic) fields, we can take advantage of a powerful formalism of Floquet theory [29], which enables us to study instead an equivalent "stationary" time independent problem. (As we will see shortly, the time variable plays the role of an additional coordinate here.) The fundamental advantage of Floquet theory consists of the fact that it enables us to introduce the concept of laser induced resonances of an atom, and thus to exploit subsequently the powerful formalism of NHQM in order to study laser induced processes in atoms.

The following theorem is what motivates us to investigate the Floquet formalism:

Theorem 4. *Let the function $\varphi : \mathbb{R}^2 \to \mathbb{C}$ and the quantity $E^{QE} \in \mathbb{C}$ satisfy the following equation:*

$$\left(\hat{H}_{\mathrm{AG}}(t') - i\hbar\partial_{t'}\right)\varphi(t', x) = E^{\mathrm{QE}}\varphi(t', x) \quad ; \tag{3.45}$$

then the function

$$\psi(t, x) \coloneqq e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t}\varphi(t', x)\Big|_{t'=t} \tag{3.46}$$

satisfies the TDSE (3.43).

Proof.

$$\begin{aligned}
\left(\hat{H}_{\mathrm{AG}}(t') - i\hbar\partial_{t'}\right)\varphi(t', x) &= E^{\mathrm{QE}}\varphi(t', x) \quad \Big| e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'} \cdot \\
E^{\mathrm{QE}}e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'}\varphi(t', x) + i\hbar e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'}\partial_{t'}\varphi(t', x) &= \hat{H}_{\mathrm{AG}}(t')e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'}\varphi(t', x) \\
i\hbar\partial_{t'}e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'}\varphi(t', x) &= \hat{H}_{\mathrm{AG}}(t')e^{-\frac{i}{\hbar}E^{\mathrm{QE}}t'}\varphi(t', x) \\
\Rightarrow i\hbar\partial_t\psi(t, x) &= \hat{H}_{\mathrm{AG}}(t)\psi(t, x) \quad .
\end{aligned}$$

□

This means that the desired solutions to the TDSE (3.43) can be obtained by solving the Floquet problem (3.45), which can be understood as an eigenvalue problem of the generalized Hamiltonian

$$\hat{\mathcal{H}}_{\mathrm{F}} \coloneqq \hat{H}_{\mathrm{AG}}(t') - i\hbar\partial_{t'} \quad ; \tag{3.47}$$

called the ***Floquet Hamiltonian***. The term $-i\hbar\partial_{t'}$ is called the kinetic operator for t. From now on, we will denote the dynamical coordinate t' as t, since there will be no possibility for confusion.

3.4.2 Basic Framework

Let us now systematically introduce the Floquet formalism. Equation (3.45) can be redisplayed as

$$\boxed{\hat{\mathcal{H}}_{\mathrm{F}}\varphi(t,x) = E^{\mathrm{QE}}\varphi(t,x)} \quad ; \tag{3.48}$$

and, as we recall, it can be understood as an eigenvalue problem of $\hat{\mathcal{H}}_{\mathrm{F}}$. The quantity E^{QE} is the so-called ***quasi-energy***. Since the Hamiltonian (3.44) is time periodic with the period of one optical cycle equal to $T = \frac{2\pi}{\omega}$, it is natural to impose on the Floquet eigenvectors $\varphi(t,x)$ the periodic boundary condition

$$\varphi(t,x) = \varphi(t+T,x) \quad ; \quad T = \frac{2\pi}{\omega} \quad ; \tag{3.49}$$

where ω is the frequency of the laser. Meaning that $\varphi(t,x)$ is ***time periodic*** with the period T. Since, in this case, time ***t is treated as an additional degree of freedom*** (dynamical coordinate), the eigenvectors of $\hat{\mathcal{H}}_{\mathrm{F}}$ belong to the vector space $L^2((0,T)\times\mathbb{R})$ (as opposed to just $L^2(\mathbb{R})$ for eigenvectors of $\hat{H}$). The eigenstates of $\hat{\mathcal{H}}_{\mathrm{F}}$ are called ***Floquet states***. We say that these atomic states are ***dressed by laser light***.

The above Theorem 4 shows that every Floquet eigensolution provides a particular solution of the TDSE (3.43). It can be even shown that the general solution of the TDSE can be built up as a linear combination of all the just mentioned different linearly independent Floquet solutions [29].

3.4.3 Brillouin Zones

Separable Hamiltonian (No Laser)

For the sake of maximum clarity, we will deal first with the no-laser case. This is because we want to motivate heuristically our considerations, which will be pursued later for the case when the laser is on, and because we wish to introduce the concept of ***Brillouin zones*** and show that the zeroth Brillouin zone corresponds to the usual atomic eigenstates in the absence of the laser. When the laser is off, the Floquet eigenproblem (3.48) becomes

$$\left(\hat{H}_{\mathrm{atom}} - i\hbar\partial_t\right)\varphi(t,x) = E^{\mathrm{QE}}\varphi(t,x) \quad ; \tag{3.50}$$

where

$$\hat{H}_{\mathrm{atom}} \coloneqq -\frac{\hbar^2}{2m}\partial_{xx} + V(x) \quad ; \tag{3.51}$$

is the time independent atomic Hamiltonian, describing the atom without the influence of a laser. We will denote its eigenstates resp. eigenvalues as $\psi_\nu(x)$ resp. E_ν, i.e.

$$\hat{H}_{\text{atom}}\psi_\nu(x) = E_\nu\psi_\nu(x) \quad . \tag{3.52}$$

We can then substitute $\psi_\nu(x)$ into (3.50) for $\varphi(t,x)$, giving us

$$\left(\hat{H}_{\text{atom}} - i\hbar\partial_t\right)\psi_\nu(x) = E^{\text{QE}}\psi_\nu(x) \tag{3.53}$$

$$E^{\text{QE}} = E_\nu \quad ; \tag{3.54}$$

i.e. $\psi_\nu(x)$ solves Equation (3.50) if $E^{\text{QE}} = E_\nu$. In other words, the eigenstates of $\hat{H}_{\text{atom}}$ coincide with a particular class of the sought Floquet solutions.

Let us now try to find all the possible Floquet eigenstates. The no-laser Floquet Hamiltonian in (3.50) is separable; therefore, its eigenvalue problem reduces to two mutually independent eigenproblems: the eigenproblem of $\hat{H}_{\text{atom}}$ we have just discussed, and the eigenproblem of the kinetic operator of t

$$-i\hbar\partial_t f_n(t) = \tilde{E}_n f_n(t) \quad ; \tag{3.55}$$

$$f(t) = f(t+T) \quad ; \quad T = \frac{2\pi}{\omega} \tag{3.56}$$

the solution of which is

$$\forall n \in \mathbb{Z} \quad ; \quad \tilde{E}_n = n\hbar\omega \quad ; \quad f_n(t) = e^{\frac{i}{\hbar}\tilde{E}_n t} \quad . \tag{3.57}$$

Since the laser is off, the laser frequency ω is irrelevant physically, yet it is still instructive to explore how ω enters mathematically into our considerations. We can now find the solution to (3.50) by multiplying the solutions of (3.52) and (3.55). The resulting quasi-energy E^{QE} will be the sum of E_ν and $\tilde{E}_n$ [29]. Therefore,

$$\forall n \in \mathbb{Z} \quad ; \quad \varphi(t,x) = \psi_\nu(x)e^{in\omega t} \quad ; \quad E^{\text{QE}} = E_\nu + n\hbar\omega \quad . \tag{3.58}$$

We have thus just found explicitly all the Floquet eigenstates and expressed them using the eigenstates of the atomic Hamiltonian $\hat{H}_{\text{atom}}$. The above Equation (3.58) shows that ***E^{QE} is defined modulo $\hbar\omega$*** (with ambiguity $n\hbar\omega$). The energies are divided into so-called ***Brillouin zones*** according to the value of n. The factor $e^{in\omega t}$ is called the Brillouin factor. Analogous statements apply also for the corresponding eigenvectors.

General Hamiltonian

When we take into account the influence of the laser, the Floquet Hamiltonian $\hat{\mathcal{H}}_{\text{F}}$ ceases to be separable. But the basic argument, which was just outlined above for the separable case, remains valid.

Theorem 5. *Let $n \in \mathbb{Z}$ and let the function $\varphi : (0,T)\times\mathbb{R} \to \mathbb{C}$ and the quantity $E^{\text{QE}} \in \mathbb{C}$ satisfy Equation (3.48) with the boundary conditions (3.49). Then the function $\tilde{\varphi} : (0,T)\times\mathbb{R} \to \mathbb{C}$ and the quantity $\tilde{E}^{\text{QE}} \in \mathbb{C}$ defined as*

$$\tilde{\varphi}(t,x) \coloneqq \varphi(t,x)e^{in\omega t} \quad ; \quad \tilde{E}^{\text{QE}} \coloneqq E^{\text{QE}} + n\hbar\omega \tag{3.59}$$

satisfy the equation

$$\hat{\mathcal{H}}_{\mathrm{F}}\tilde{\varphi}(t,x) = \tilde{E}^{\mathrm{QE}}\tilde{\varphi}(t,x) \tag{3.60}$$

with the boundary conditions

$$\tilde{\varphi}(t+T,x) = \tilde{\varphi}(t,x) \quad . \tag{3.61}$$

Proof.

$$\left(\hat{H}_{\mathrm{AG}}(t) - i\hbar\partial_t\right)\tilde{\varphi}(t,x) = \tilde{E}^{\mathrm{QE}}\tilde{\varphi}(t,x) \tag{3.62}$$

$$\left(\hat{H}_{\mathrm{AG}}(t) - i\hbar\partial_t\right)\varphi(t,x)e^{in\omega t} = \left(E^{\mathrm{QE}} + n\hbar\omega\right)\left(\varphi(t,x)e^{in\omega t}\right) \tag{3.63}$$

$$\begin{aligned}\hat{H}_{\mathrm{AG}}(t)\varphi(t,x)e^{in\omega t} + n\omega\hbar\tilde{\varphi}(t,x)e^{in\omega t} - i\hbar\partial_t\varphi(t,x)e^{in\omega t} = \\ = E^{\mathrm{QE}}\varphi(t,x)e^{in\omega t} + n\omega\hbar\tilde{\varphi}(t,x)e^{in\omega t} \quad \Big| \cdot e^{-in\omega t}\end{aligned} \tag{3.64}$$

$$\left(\hat{H}_{\mathrm{AG}}(t) - i\hbar\partial_t\right)\varphi(t,x) = E^{\mathrm{QE}}\varphi(t,x) \quad . \tag{3.65}$$

□

We see that the quazi-energies are again divided into the Brillouin zones, even for the general case. At zero laser intensity the corresponding zeroth Brillouin zone states coincide with the stationary atomic eigenstates as explained above in (3.58). When the laser is continuously switched on, these atomic states change continuously as a function of α_0, in other words, they become dressed by laser light. For any laser intensity, all the other Floquet eigensolutions are constructed from those of the zeroth Brillouin zone, as detailed in (3.59).

3.4.4 The Floquet Coupled Channel Problem

General Formulation

We shall now elaborate further on the Floquet formalism. We will use the fact that functions

$$e^{in\omega t} \quad ; \quad n \in \mathbb{Z} \tag{3.66}$$

create a complete basis set, which is orthonormal with respect to the following scalar product:

$$\frac{1}{T}\int_0^T \mathrm{d}t\ \left(e^{in\omega t}\right)^*\left(e^{in'\omega t}\right) = \delta_{nn'} \quad . \tag{3.67}$$

We can, therefore, expand $\varphi(t,x)$ as

$$\varphi(t,x) = \sum_{n=-\infty}^{+\infty}\varphi_n(x)e^{in\omega t} \quad . \tag{3.68}$$

The substitution of (3.68) into (3.48) gives us

$$\left(-\frac{\hbar^2}{2m}\partial_{xx} + V(x+\alpha_0\cos(\omega t)) - i\hbar\partial_t\right)\sum_{n=-\infty}^{+\infty}\varphi_n(x)e^{in\omega t} = E^{\mathrm{QE}}\sum_{n=-\infty}^{+\infty}\varphi_n(x)e^{in\omega t} \tag{3.69}$$

$$\begin{aligned}
&-\frac{\hbar^2}{2m}\sum_{n'=-\infty}^{+\infty}\varphi_{n'}''(x)e^{in'\omega t} + V(x+\alpha_0\cos(\omega t))\sum_{n'=-\infty}^{+\infty}\varphi_{n'}(x)e^{in'\omega t} + \\
&+\hbar\omega\sum_{n'=-\infty}^{+\infty}\varphi_{n'}(x)e^{in'\omega t} = E^{\mathrm{QE}}\sum_{n'=-\infty}^{+\infty}\varphi_{n'}(x)e^{in'\omega t} \quad \Big|\int_0^T \mathrm{d}t\, e^{-in\omega t} \\
&-\frac{\hbar^2}{2m}\varphi_n''(x) + \hbar\omega n\varphi_n(x) + \sum_{n'=-\infty}^{+\infty}V_{nn'}(x)\varphi_{n'}(x) = E^{\mathrm{QE}}\varphi_n(x) \quad ;
\end{aligned} \tag{3.70}$$

where

$$\begin{aligned}
V_{nn'} &:= \frac{1}{T}\int_0^T e^{-in\omega t}V(x+\alpha_0\sin(\omega t))e^{in'\omega t}\,\mathrm{d}t = \\
&= \frac{1}{T}\int_0^T V(x+\alpha_0\cos(\omega t))e^{-i(n-n')\omega t}\,\mathrm{d}t =: V_{n-n'}(x) \quad .
\end{aligned} \tag{3.71}$$

For more compact formulation, let us now express these equations in the language of matrices:

$$\vec{\varphi}(x) := \begin{pmatrix} \vdots \\ \varphi_1(x) \\ \varphi_0(x) \\ \varphi_{-1}(x) \\ \vdots \end{pmatrix} \quad ; \tag{3.72}$$

$$\begin{pmatrix} \ddots & & & & \iddots \\ & \bullet & V_1(x) & V_2(x) & V_3(x) & \\ & V_{-1}(x) & \bullet & V_1(x) & V_2(x) & \\ & V_{-2}(x) & V_{-1}(x) & \bullet & V_1(x) & \\ & V_{-3}(x) & V_{-2}(x) & V_{-1}(x) & \bullet & \\ \iddots & & & & & \ddots \end{pmatrix}\begin{pmatrix} \vdots \\ \varphi_1(x) \\ \varphi_0(x) \\ \varphi_{-1}(x) \\ \vdots \end{pmatrix} = E\begin{pmatrix} \vdots \\ \varphi_1(x) \\ \varphi_0(x) \\ \varphi_{-1}(x) \\ \vdots \end{pmatrix} \quad ; \tag{3.73}$$

where the diagonal term ($\bullet$) in the nth row and nth column is

$$-\frac{\hbar^2}{2m}\partial_{xx} + n\hbar\omega + V_0(x) \quad . \tag{3.74}$$

The problem (3.70) can then be concisely written as

$$\boxed{-\frac{\hbar^2}{2m}\partial_{xx}\vec{\varphi}(x) + \underline{\underline{\mathcal{V}}}(x)\vec{\varphi}(x) = E^{\mathrm{QE}}\vec{\varphi}(x)} \quad ; \tag{3.75}$$

$$[\mathcal{V}(x)]_{nn'} := V_{n-n'}(x) + \delta_{nn'}n\hbar\omega \quad . \tag{3.76}$$

This equation formally resembles the 1D time independent Schrödinger equation, the only difference consists in the fact that the eigenfunctions have multiple components and that the potential is a matrix entity. Equation (3.75) is called the ***coupled channel Schrödinger equation*** (or the coupled channel problem). Its different rows and columns are called ***channels***.

Weak Field

From now on we will assume a weak intensity field, meaning that

$$\hat{H}_{\mathrm{AG}}(t) = -\frac{\hbar^2}{2m}\partial_{xx} + V(x) + V'(x)\alpha_0 \cos(\omega t) \quad . \tag{3.77}$$

The elements of $\underline{\underline{\mathcal{V}}}(x)$ then take the following form:

$$\forall n, n' \in \mathbb{Z} \quad ; \quad V_{n-n'}(x) = V(x)\delta_{n-n'} + V'(x)\alpha_0 \frac{1}{2i}(\delta_{(n-n'+1)0} - \delta_{(n-n'-1)0}) \quad ; \tag{3.78}$$

which can be written out for different values of $n - n'$ as

$$V_0(x) = V(x) \quad ; \tag{3.79}$$

$$V_1(x) = -V'(x)\alpha_0 \frac{1}{2i} = V_{-1}^*(x) \quad ; \tag{3.80}$$

$$\forall k \in \mathbb{Z}, |k| > 1 \quad ; \quad V_k(x) = 0 \quad . \tag{3.81}$$

The matrix $\underline{\underline{\mathcal{V}}}(x)$, therefore, becomes tridiagonal. Equation (3.75) is in this case called the ***tridiagonal Floquet problem***. Without the laser, this matrix would be diagonal,

$$V_{n-n'}(x) = V(x)\delta_{nn'} \quad ; \tag{3.82}$$

and we could therefore separate the individual channels. In other words, the channels would then be independent, and n would thus become a good quantum number.

3.4.5 Nonhermitian Floquet theory

Let us analyze again the above formulated Floquet formalism. The diagonal of the Floquet matrix possesses the form $\hat{H}_{\mathrm{atom}} + n\hbar\omega$, where $\hat{H}_{\mathrm{atom}}$ denotes the Hamiltonian describing the atom without the influence of a laser defined in (3.51). The Floquet channels are ***mutually shifted by $n\hbar\omega$***, and the off-diagonal matrix elements represent the couplings generated by the laser. These are however spatially localized (in the acceleration gauge), they die out for large values of $|x|$. This shows that the nth diagonal channel is locally (for finite values of x) coupled by the laser to the other channels.

In the absence of laser light, any bound state of the nth channel is embedded in the continuum of the lower lying channels $n' < n$. Now, if the laser is turned on, this bound state becomes coupled to the just mentioned continuum states, and ceases to be bound, i.e. it becomes a metastable state called a ***Feshbach resonance*** [29].

HQM does not offer an efficient language for describing resonances, as we have seen in Chapters 1-2. Therefore, if resonances are present, we are motivated

to formulate nonhermitian Floquet theory. We will use complex scaling for this purpose, but omit all the underlying technical details, which are similar to those described in Section 2.2 above. Since t is a periodic coordinate and as such won't cause divergence of the wavefunctions, it will only be necessary to scale the space coordinate x. The passage into nonhermitian Floquet theory is facilitated via performing the following substitution:

$$x \mapsto xe^{i\theta} \quad ; \quad \theta \in (\arg(\sqrt{2mE^{\mathrm{QE}}}), \frac{\pi}{2}) \quad ; \tag{3.83}$$

as explained in Subsection 2.2.5. Correspondingly, our complex scaled Floquet eigenproblem will look as follows:

$$\hat{\mathcal{H}}_{\mathrm{F}}^{\theta}\varphi^{\theta}(t,x) = E_{\theta}^{\mathrm{QE}}\varphi^{\theta}(t,x) \quad ; \tag{3.84}$$

where

$$\hat{\mathcal{H}}_{\mathrm{F}}^{\theta} \coloneqq -\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta}) + V'(xe^{i\theta})\alpha_0\cos(\omega t) - i\hbar\partial_t \quad ; \tag{3.85}$$

$$\varphi^{\theta}(t+T,x) = \varphi^{\theta}(t,x) \quad . \tag{3.86}$$

The eigenproblem (3.75) is transformed into

$$\boxed{-\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx}\vec{\varphi^{\theta}}(x) + \underline{\underline{\mathcal{V}}}^{\theta}(x)\vec{\varphi^{\theta}}(x) = E_{\theta}^{\mathrm{QE}}\vec{\varphi^{\theta}}(x)} \quad ; \tag{3.87}$$

where

$$\vec{\varphi^{\theta}}(x) \coloneqq \begin{pmatrix} \vdots \\ \varphi_1^{\theta}(x) \\ \varphi_0^{\theta}(x) \\ \varphi_{-1}^{\theta}(x) \\ \vdots \end{pmatrix} \quad ; \tag{3.88}$$

$$\underline{\underline{\mathcal{V}}}^{\theta}(x) \coloneqq \begin{pmatrix} \ddots & & \iddots \\ & -\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta}) + 0\hbar\omega & \frac{\alpha_0}{2}V'(xe^{i\theta}) & \\ & \frac{\alpha_0}{2}V'(xe^{i\theta}) & -\frac{\hbar^2}{2m}e^{-2i\theta}\partial_{xx} + V(xe^{i\theta}) + 1\hbar\omega & \\ \iddots & & & \ddots \end{pmatrix} \quad . \tag{3.89}$$

This corresponds to our nonhermitian Floquet problem. It can be shown, analogically to the proof of Theorem 2 in Chapter 2, that the resulting resonance eigenvalues are independent of θ. The corresponding Floquet resonances (metastable atomic states dressed by laser light) can be then in principle obtained by solving this complex scaled coupled channel problem numerically, using the basis set expansion method and linear algebra, much as we did already in Chapter 2. Subsequently, the associated solution of the TDSE can be accessed via Equation (3.46), and physical observables can be calculated (we omit here all the details and refer to [29]).

An example calculation of this sort is presented in the following figure:

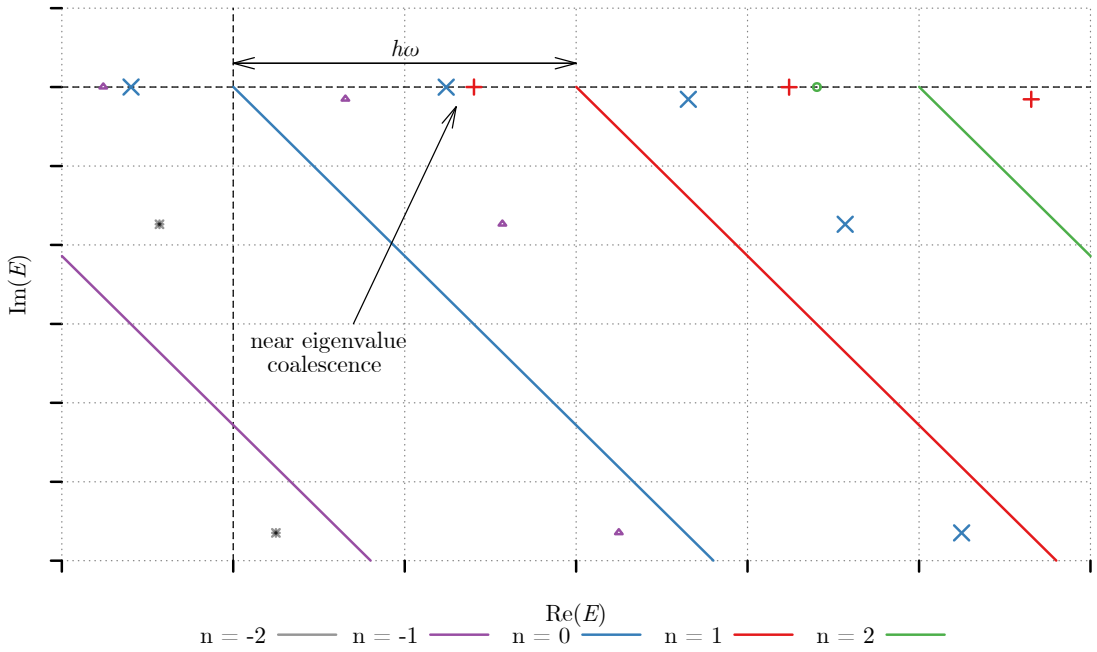

Figure 3.1: Eigenvalues of the complex scaled Floquet eigenproblem (3.87) plotted schematically for $\theta = 0.2$, with the toy potential (1.73), and without the presence of the laser ($\omega \neq 0, \alpha_0 = 0$). Different colors (violet, blue, red, green) correspond to the different Brillouin zones whose pertinent values of n are indicated in the figure. The "blue" eigenvalues associated with the $n = 0$ Brillouin zone are arising from those plotted in Figure 2.1 in Chapter 2 where we considered just an atomic system without coupling to the laser. The "violet", "red", and "green" eigenvalues are constructed from their "blue" counterparts via mere shift by $n\hbar\omega$, consistently with what we have proven above in Equation (3.59). As one can see, the Floquet resonances associated with different Brillouin zones are mixed together in the complex energy plane, and some of them can get even very close to each other (see, e.g. the blue and red crosses marked by the arrow). The red cross arises in this case from the $n = 1$ bound state of our model atom, whereas the blue cross originates from the first $n = 0$ shape type atomic resonance (whose width Γ is so small that this resonance is located almost at the real axis). This also shows that the just shown Floquet resonances are of a mixed shape-Feshbach type.

3.5 Nonhermitian Degeneracy - Exceptional Points Induced by Laser

3.5.1 Theoretical Considerations

So far, the laser parameters α_0 and ω have been completely arbitrary. These are two independent control parameters, enabling us to shift the resonance energies in any direction of the 2D complex plane.

This brings us to an idea to optimize the laser parameters (α_0, ω) as to arrange for a nonhermitian degeneracy, the so-called ***exceptional point*** (EP) (This

amounts, e.g. to arrange for coalescence of the red and the blue cross plotted in Figure 3.1.).

Let us describe now the formation of an EP explicitly. We will use here the bound state and resonance energy values calculated, without the presence of a laser, in Chapter 2, using the toy potential (1.73), displayed in Table 2.1 as well as their corresponding statefunctions, plotted in Figures 2.3-2.4. The resonances, the energies of which we'll try to match, are the first $n = 0$ Feshbach type resonance (red cross) and the $n = 1$ Brillouin resonance (blue cross). The eigenvalue associated with the first $n = 0$ shape type resonance, for $\alpha_0 = 0$, is

$$E_{\rm R} =: \mathcal{E}_{\rm R} - \frac{i}{2}\Gamma_{\rm R} = 0.62097 - 5.82666 \cdot 10^{-5} i \quad ; \tag{3.90}$$

and its corresponding eigenfunction $\psi^{\theta}_{\rm R}(x)$. Recall that we use arbitrary units throughout. The eigenvalue associated with the $n = 1$ Brillouin resonance, arising form the original atomic bound state shifted by $\hbar\omega$, equals to

$$E_{\rm B} =: \mathcal{E}_{\rm B} + \hbar\omega = -0.29796 + \hbar\omega \quad ; \tag{3.91}$$

and its corresponding complex scaled eigenfunction will be denoted as $\psi^{\theta}_{\rm B}(x)e^{i\omega t}$.

When the laser is switched on, the original bound state penetrates into the negative imaginary energy plane, and the different Brillouin zones of Figure 3.1 become coupled. This results in shifting the locations of the Floquet resonances in the complex energy plane. Importantly, the largest laser induced coupling occurs here in the case of those Floquet resonances which are nearly degenerate in the absence of the laser. This allows us, to a good approximation, to investigate the formation of an EP just via taking into account the two above mentioned Floquet states $\psi^{\theta}_{\rm R}(x), \psi^{\theta}_{\rm B}(x)e^{i\omega t}$ and their laser induced coupling. Here we neglect the couplings to other Floquet resonances as well as to the rotated continua. In other words, we use from now on the truncated Floquet basis set $(\psi^{\theta}_{\rm R}, \psi^{\theta}_{\rm B}(x)e^{i\omega t})$. This reduces the matrix (3.89) to

$$\begin{pmatrix} (\psi^{\theta}_{\rm R}|\hat{\mathcal{H}}^{\theta}_{\rm F}|\psi^{\theta}_{\rm R}) & (\psi^{\theta}_{\rm R}|V'(xe^{i\theta})\frac{\alpha_0}{2}|\psi^{\theta}_{\rm B}) \\ (\psi^{\theta}_{\rm B}|V'(xe^{i\theta})\frac{\alpha_0}{2}|\psi^{\theta}_{\rm R}) & (\psi^{\theta}_{\rm B}|\hat{\mathcal{H}}^{\theta}_{\rm F}|\psi^{\theta}_{\rm B}) \end{pmatrix} = \begin{pmatrix} \mathcal{E}_{\rm R} - \frac{i}{2}\Gamma_R & \alpha_0\mathcal{D} \\ \alpha_0\mathcal{D} & \mathcal{E}_{\rm B} + \hbar\omega \end{pmatrix} =: \underline{\underline{\mathcal{H}}} \quad ; \tag{3.92}$$

where the coupling element $\mathcal{D} \coloneqq \frac{1}{2}(\psi^{\theta}_{\rm R}|V'(xe^{i\theta})|\psi^{\theta}_{\rm B}) =: \mathcal{D}_{\rm Re} + i\mathcal{D}_{\rm Im}$ can be obtained numerically, as

$$\mathcal{D} = \frac{1}{2}(\psi^{\theta}_{\rm R}|V'(xe^{i\theta})|\psi^{\theta}_{\rm B}) \approx \int_{-25}^{25} {\rm d}x\, \psi^{\theta}_{\rm R}(x)V'(xe^{i\theta})\psi^{\theta}_{\rm B}(x) = -1.24145 + 2.95759 \cdot 10^{-4} i \quad ; \tag{3.93}$$

It can be shown by contour integration that the value of $\mathcal{D}$ is not dependent on θ. Recall that we are looking for values of (ω, α_0) such that quasi-energy degeneracy occurs. For this purpose we will first find the eigenvalues of (3.92).

To help us further simplify this problem, the matrix $\underline{\underline{\mathcal{H}}}$ can be rewritten as

$$\underline{\underline{\mathcal{H}}} = A\underline{\underline{I}} + B \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix} \quad ; \tag{3.94}$$

where

$$A = \frac{1}{2}(\mathcal{E}_{\mathrm{R}} + \mathcal{E}_{\mathrm{B}} + \hbar\omega) - \frac{i}{4}\Gamma_R \quad ; \tag{3.95}$$

$$B = \frac{1}{2}(\mathcal{E}_{\mathrm{R}} - \mathcal{E}_{\mathrm{B}} - \hbar\omega) - \frac{i}{4}\Gamma_R \quad ; \tag{3.96}$$

$$\lambda = \frac{2\mathcal{D}_{\mathrm{Re}}(\mathcal{E}_{\mathrm{R}} - \mathcal{E}_{\mathrm{B}} - \hbar\omega) - \mathcal{D}_{\mathrm{Im}}\Gamma_R + i\left[2\mathcal{D}_{\mathrm{Im}}(\mathcal{E}_{\mathrm{R}} - \mathcal{E}_{\mathrm{B}} - \hbar\omega) + \mathcal{D}_{\mathrm{Re}}\Gamma_R\right]}{(\mathcal{E}_{\mathrm{R}} - \mathcal{E}_{\mathrm{B}} - \hbar\omega)^2 + \frac{1}{4}\Gamma_R^2}\alpha_0 \quad . \tag{3.97}$$

Since the eigenvalues of $\underline{\underline{\mathcal{H}}}$ can, thanks to Equation (3.94), be obtained as the sum of A and the eigenvalues of the matrix

$$\begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix} \quad ; \tag{3.98}$$

the eigenproblem (3.94) is reduced to solving the eigenvalue problem of (3.98), which is done in Appendix D. Namely, the resulting eigenvalues of $\underline{\underline{\mathcal{H}}}$ are

$$E_{\pm}(\lambda) = A \pm \sqrt{\lambda^2 + 1} \quad . \tag{3.99}$$

The just displayed formula (3.99) shows immediately that finding the desired special values of (ω, α_0) is possible. Indeed, an ***eigenvalue degeneracy*** occurs whenever

$$\lambda = \pm i \quad . \tag{3.100}$$

And the sought EP is thus formed.

Let us consider specifically the case of $\lambda = i$. By substituting $\lambda = i$ into (3.95)-(3.97), we can calculate the values of (ω, α_0) corresponding to this EP as

$$\boxed{\boldsymbol{\omega_{\mathrm{EP}} = \frac{1}{\hbar}\left(\mathcal{E}_{\mathrm{R}} - \mathcal{E}_{\mathrm{B}} - \frac{1}{2}\frac{\mathcal{D}_{\mathrm{Im}}}{\mathcal{D}_{\mathrm{Re}}}\Gamma_{\mathrm{R}}\right)} \quad ;} \tag{3.101}$$

$$\boxed{\boldsymbol{\alpha_{0\mathrm{EP}} = \frac{1}{4}\frac{\Gamma_{\mathrm{R}}}{\mathcal{D}_{\mathrm{Re}}}} \quad .} \tag{3.102}$$

3.5.2 Numerical Calculation

We will now again employ the toy potential (1.73), while setting $\hbar = 1$, $m = 1$ and using arbitrary units, to numerically calculate the values of $(\omega_{\mathrm{EP}}, \alpha_{0\mathrm{EP}})$. We make use of the values of the resonance and bound state energies calculated in Section 2.2. This gives us the parameters causing the creation of an EP by laser:

$$\boxed{\boldsymbol{\omega_{\mathrm{EP}} = 0.91893} \quad ;} \tag{3.103}$$

$$\boxed{\boldsymbol{\alpha_{0\mathrm{EP}} = 9.38682 \cdot 10^{-5}}} \quad . \tag{3.104}$$

We see that the value α_0 is indeed small enough compared to the lengthscale of the used potential (1.73). Hence the weak field approximation (3.77) is well justified.

3.5.3 Properties of the Exceptional Points

In Appendix D, we have shown that as λ approaches $\pm i$, the eigenvectors of (3.98) start overlapping and become more linearly dependent, eventually resulting in an ***eigenvector degeneracy*** for $\lambda = \pm i$. The phenomenon of eigenvector degeneracy has been known mathematically in linear algebra (defective matrices, Jordan blocs). The degeneracy (coalescence) of eigenvectors is a phenomenon specific for NHQM, it does not have an analogy in standard HQM. This is where the terminology "exceptional points" comes from. The resulting single eigenvector of (3.98) is

$$\begin{pmatrix} 1 \\ \pm i \end{pmatrix} \quad . \tag{3.105}$$

This vector is self orthogonal in respect to the C-product (2.62).

Interesting mathematical properties of the EPs include an unusual closure property (see Equation (D.17) in the Appendix D), self orthogonality as already mentioned above and as detailed in Appendix D, as well as double valuedness of the eigenvalue when encircling an EP. This double valuedness is illustrated in the figure below:

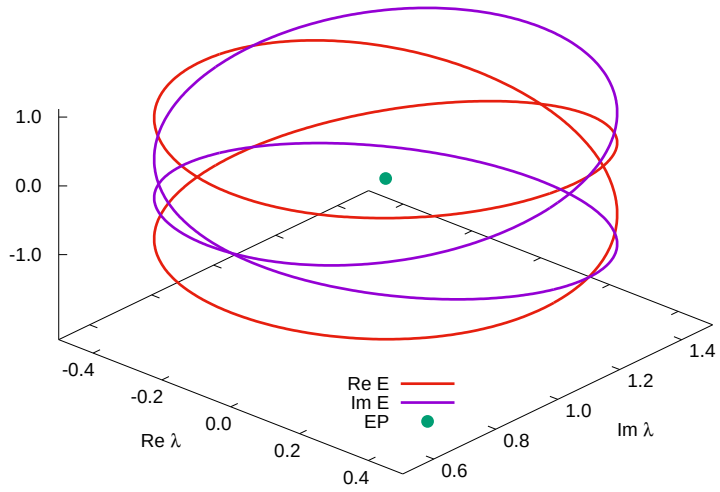

Figure 3.2: Real and imaginary parts of the function $\sqrt{\lambda^2+1}$ entering into the eigenvalue formula (3.98). For convenience, we plot here just a segment of the graph, corresponding to $\lambda = +i + e^{+i\beta}$ where $\beta \in [0, 4\pi)$. As one can see, the plotted graph of $\sqrt{\lambda^2+1}$ is ***double valued***, i.e. an EP $\lambda = +i$ must be ***encircled twice*** (β must run from 0 to 4π) in order to return to the starting value associated with $\beta = 0$.

Most importantly, the EPs are not just exotic mathematical peculiarities. In fact, just the opposite is true: EPs arise in a wide variety of physically relevant situations (e.g. quantum mechanics of laser driven atoms [4], [6], [21], [23], [24], [31], waveguide optics [13], acoustics [34], electric circuit theory [7], elasticity [35], excited state quantum phase transitions [39]). The physical implications of EPs represent

an active area of current research, one may expect significant discoveries coming in the future.

3.6 Summary

In this Chapter 3 we have provided a tutorial overview of the problem of interaction of an atom with laser. We have introduced an adequate Hamiltonian in different mutually equivalent gauges (namely, the momentum, reduced momentum, length, and acceleration gauges), and highlighted the advantage of the acceleration gauge for theoretical studies of laser assisted scattering phenomena.

Subsequently, we have considered more specifically just monochromatic lasers, and formulated the powerful formalism of the ***Floquet theory***, which enables us to formulate laser driven atomic dynamics as e generalized stationary eigenvalue problem (where the time variable plays the role of an additional coordinate).

Importantly, the Floquet picture clarifies how ***laser induced resonances*** arise in atomic systems. Nonhermitian complex scaled Floquet theory was thus accordingly introduced.

The just summarized powerful theoretical tools enable us to study the creation of a nonhermitian degeneracy known as an ***exceptional point*** (EP). We have explicitly shown how such an EP is formed by choosing appropriately the laser parameters, and we have commented on peculiar mathematical and physical properties of EPs.

Concluding Remarks

In this Bachelor project, we have outlined (in a more or less self contained fashion) the formalism of ***nonhermitian quantum mechanics*** (NHQM) and its application on ***scattering theory***. Explicit numerical calculations (for a simple yet ubiquitous 1D toy model) have illustrated the strength of NHQM. It has also been verified that the two existing distinct approaches to NHQM (***complex scaling***, ***method Siegert pseudostates***) provide the same physical information as the conventional scattering calculations. Being equipped with the powerful formalism of NHQM, we have presented in more detail one of its most prominent applications related to laser driving of atoms. Most importantly, an emergence of a nonhermitian degeneracy called an ***exceptional point*** (EP) has been demonstrated theoretically for the case of laser driven atoms, parameters characterizing such an EP have been also explicitly calculated, and we have commented on peculiar mathematical and physical properties of the EPs.

I believe that the contents of this project may serve as a reasonable starting point to anyone who wishes to enter the turbulently evolving field of NHQM.

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Appendix A

LSE Vectors $\left|\psi^{\pm}_{E\eta}\right\rangle$ as Solutions to the Schrödinger Equation

Proof. Let $\epsilon \to 0^+$ and let $\left|\psi^{\pm}_{E\eta}\right\rangle$ satisfy the Lippmann-Schwinger equation, then

$$\left|\psi^{\pm}_{E\eta}\right\rangle = \left|\phi_{E\eta}\right\rangle + \lim_{\epsilon\to 0^+} \frac{1}{E - \hat{H} \pm i\epsilon}\hat{V}\left|\phi_{E\eta}\right\rangle \quad \Big|(E - \hat{H} \pm i\epsilon)\cdot$$
$$(E - \hat{H})\left|\psi^{\pm}_{E\eta}\right\rangle \pm i\epsilon\left|\psi^{\pm}_{E\eta}\right\rangle = (E - \hat{H})\left|\phi_{E\eta}\right\rangle \pm i\epsilon\left|\phi_{E\eta}\right\rangle + \hat{V}\left|\phi_{E\eta}\right\rangle \quad ;$$

and since $\hat{H} = \hat{H}_0 + \hat{V}$ and $\epsilon \to 0^+$

$$(E - \hat{H})\left|\psi^{\pm}_{E\eta}\right\rangle \pm i\epsilon\left|\psi^{\pm}_{E\eta}\right\rangle = (E - \hat{H}_0)\left|\phi_{E\eta}\right\rangle \pm i\epsilon\left|\phi_{E\eta}\right\rangle$$
$$(E - \hat{H})\left|\psi^{\pm}_{E\eta}\right\rangle = (E - \hat{H}_0)\left|\phi_{E\eta}\right\rangle = |0\rangle$$
$$\hat{H}\left|\psi^{\pm}_{E\eta}\right\rangle = E\left|\psi^{\pm}_{E\eta}\right\rangle \quad .$$

□

Appendix B

Probability Conservation in Scattering

Proof. By applying $\int_{-L}^{L} \mathrm{d}x \left(\tilde{\psi}^{+}\right)^{*}$ for large enough L to both sides of (1.41) we get

$$\int_{-L}^{L} \mathrm{d}x \left(\tilde{\psi}^{+}\right)^{*}(x)\left(-\frac{\hbar^2}{2m}\partial_{xx}+V(x)\right)\psi^{+}(x) = E\int_{-L}^{L} \mathrm{d}x \left(\tilde{\psi}^{+}\right)^{*}(x)\tilde{\psi}^{+}(x) \quad ;$$

$$\int_{-L}^{L} \mathrm{d}x\, \tilde{\psi}^{+}(x)\left(-\frac{\hbar^2}{2m}\partial_{xx}+V(x)\right)\left(\tilde{\psi}^{+}\right)^{*}(x) = E\int_{-L}^{L} \mathrm{d}x\, \tilde{\psi}^{+}(x)\left(\tilde{\psi}^{+}\right)^{*}(x) \quad ;$$

$$\int_{-L}^{L} \mathrm{d}x \left[-\left(\tilde{\psi}^{+}\right)^{*}(x)\partial_{xx}\tilde{\psi}^{+}(x)+\tilde{\psi}(x)+\partial_{xx}\left(\tilde{\psi}^{+}\right)^{*}\right] = 0 \quad ;$$

$$\left[\tilde{\psi}^{+}(x)\partial_x\left(\tilde{\psi}^{+}\right)^{*}(x)-\left(\tilde{\psi}^{+}\right)^{*}(x)\partial_x\tilde{\psi}^{+}(x)\right]\Big|_{-L}^{L} = 0 \quad .$$

Since L is as large as one wishes, we can now use the boundary conditions (1.42)-(1.43) to get

$$\begin{aligned} iK\left[-|T(E)|^2-|T(E)|^2+1-e^{2iKL}R(E)+e^{-2iKL}R(E)-|R(E)|^2+\right. & \\ \left.+1-e^{-2iKL}R(E)+e^{2iKL}R(E)-|R(E)|^2\right] &= 0 \quad ; \\ 2\left[|R(E)|^2+|T(E)|^2-1\right] &= 0 \quad ; \\ |R(E)|^2+|T(E)|^2 &= 1 \quad . \end{aligned}$$

□

Appendix C

Nonexistence of Siegert States with $K \in \mathbb{R}\backslash\{0\}$

Proof. Let us assume that $K \in \mathbb{R}$, $K \neq 0$.

$$K_2 = 0 \Rightarrow \psi\left(x \to \pm\infty\right) = e^{\pm iK_1 x} \quad .$$

Equation (2.1) for ψ and ψ^* tells us that

$$\begin{aligned} -\frac{\hbar^2}{2m}\partial_{xx}\psi(x) + V(x)\psi(x) &= E\psi(x) \quad \Big|\psi^*(x) \quad ; \\ -\frac{\hbar^2}{2m}\partial_{xx}\psi^*(x) + V(x)\psi^*(x) &= E^*\psi^*(x) \quad \Big|\psi(x) \end{aligned}$$

$$\begin{aligned} -\frac{\hbar^2}{2m}\partial_{xx}\psi(x)\psi^*(x) + V(x)\psi(x)\psi^*(x) &= E\psi(x)\psi^*(x) \quad ; \\ -\frac{\hbar^2}{2m}\partial_{xx}\psi^*(x)\psi(x) + V(x)\psi^*(x)\psi(x) &= E^*\psi^*(x)\psi(x) \end{aligned}$$

$$\begin{aligned} -\frac{\hbar}{2m}\left[\psi^*(x)\psi''(x) - \psi(x)\left(\psi^*\right)'(x)\right] = 0 \quad \Big| \int_a^b \mathrm{d}x \quad ; \\ \left[\psi^*(x)\psi''(x) - \psi(x)\left(\psi^*\right)'(x)\right]\Big|_a^b = 0 \quad ; \end{aligned}$$

where $W_\psi(x) \coloneqq \psi^*(x)\psi''(x) - \psi(x)\left(\psi^*\right)'(x)$ is the Wronskian of ψ, i.e $W_\psi(x)$ is x-independent (flux conservation).

Now for L large enough and

$$a \coloneqq -L, \quad b \coloneqq L \quad ;$$

$$\begin{aligned} \left[\psi^*(x)\psi''(x) - \psi(x)\left(\psi^*\right)'(x)\right]\Big|_{-L}^{L} &= 0 \\ K_1\left[-K_1 + i + K_1 + i\right] &= 0 \\ i2K_1 &= 0 \\ K_1 &= 0 \quad . \end{aligned}$$

meaning that $K = 0$, which contradicts our initial assumption. Therefore, a situation where $K \in \mathbb{R}\backslash\{0\}$ is impossible. □

Appendix D

Solution to the Eigenvalue Problem of (3.98)

Let us denote

$$\underline{\underline{H_\lambda}} \coloneqq \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix} \quad ; \tag{D.1}$$

where $\lambda \in \mathbb{C}$. We shall now solve the eigenvalue problem of $\underline{\underline{H_\lambda}}$

$$\underline{\underline{H_\lambda}} \vec{\psi}_\lambda^{(j)} = E_\lambda^{(j)} \vec{\psi}_\lambda^{(j)} \quad ; \tag{D.2}$$

which can be expressed in the following way

$$\det\left(\underline{\underline{H_\lambda}} - \hat{I}E\right) = \begin{vmatrix} 1 - E_\lambda^{(j)} & \lambda \\ \lambda & -1 - E_\lambda^{(j)} \end{vmatrix} = -\left(1 - E_\lambda^{(j)}\right)^2 - \lambda^2 = 0 \quad . \tag{D.3}$$

Therefore, the eigenvalues of $\underline{\underline{H_\lambda}}$ are

$$\boldsymbol{E_\lambda^{\pm 1} = \pm\sqrt{\lambda^2 + 1}} \quad . \tag{D.4}$$

D.1 Non-degenerate Case

Let us first investigate the situation, when

$$\lambda \neq \pm i \quad ; \tag{D.5}$$

and therefore

$$E_\lambda^{(\pm 1)} \neq 0 \Rightarrow E_\lambda^{(+1)} \neq E_\lambda^{(-1)} \quad . \tag{D.6}$$

The eigenvectors of $\underline{\underline{H_\lambda}}$ can be found as:

$$\begin{pmatrix} 1 - E_\lambda^{(+1)} & \lambda \\ \lambda & -1 - E_\lambda^{(+1)} \end{pmatrix} = \begin{pmatrix} 1 - \sqrt{\lambda^2+1} & \lambda \\ \lambda & -1 - \sqrt{\lambda^2+1} \end{pmatrix} \sim$$
$$\sim \begin{pmatrix} -\lambda^2 & \lambda\left(1 + \sqrt{\lambda^2+1}\right) \\ \lambda^2 & -\lambda\left(1 + \sqrt{\lambda^2+1}\right) \end{pmatrix} \sim \begin{pmatrix} -\lambda & 1 + \sqrt{\lambda^2+1} \\ 0 & 0 \end{pmatrix}$$
$$\Rightarrow \boldsymbol{\vec{\psi}_\lambda^{(+1)} = C_\lambda^{(+1)} \begin{pmatrix} 1 + \sqrt{\lambda^2+1} \\ \lambda \end{pmatrix}} \quad . \tag{D.7}$$

$$\begin{pmatrix} 1-E_\lambda^{(-1)} & \lambda \\ \lambda & -1-E_\lambda^{(-1)} \end{pmatrix} = \begin{pmatrix} 1+\sqrt{\lambda^2+1} & \lambda \\ \lambda & -1+\sqrt{\lambda^2+1} \end{pmatrix} \sim$$
$$\sim \begin{pmatrix} \lambda\left(1+\sqrt{\lambda^2+1}\right) & \lambda^2 \\ \lambda\left(1+\sqrt{\lambda^2+1}\right) & \lambda^2 \end{pmatrix} \sim \begin{pmatrix} 1+\sqrt{\lambda^2+1} & \lambda \\ 0 & 0 \end{pmatrix}$$
$$\Rightarrow \boldsymbol{\vec{\psi}_\lambda^{(-1)} = C_\lambda^{(-1)} \begin{pmatrix} -\lambda \\ 1+\sqrt{\lambda^2+1} \end{pmatrix}} \quad . \tag{D.8}$$

We will now show that with the appropriate normalization the resulting linearly independent eigenvectors are orthonormal:

$$\left(\vec{\psi}_\lambda^{(1)}\right)^\intercal \vec{\psi}_\lambda^{(-1)} = \left(\vec{\psi}_\lambda^{(-1)}\right)^\intercal \vec{\psi}_\lambda^{(1)} =$$
$$= C_\lambda^{(1)} C_\lambda^{(-1)} \left[-\lambda\left(1+\sqrt{\lambda^2+1}\right) + \lambda\left(1+\sqrt{\lambda^2+1}\right)\right] = 0$$
$$\left(\vec{\psi}_\lambda^{(1)}\right)^\intercal \vec{\psi}_\lambda^{(1)} = \left(C_\lambda^{(1)}\right)^2 \left(1+\sqrt{\lambda^2+1}^2+\lambda^2\right) = 2\left(C_\lambda^{(1)}\right)^2 \left(\lambda^2+\sqrt{\lambda^2+1}+1\right)$$
$$\left(\vec{\psi}_\lambda^{(-1)}\right)^\intercal \vec{\psi}_\lambda^{(-1)} = 2\left(C_\lambda^{(-1)}\right)^2 \left(\lambda^2+\sqrt{\lambda^2+1}+1\right)$$
$$\lambda^2+\sqrt{\lambda^2+1}+1 = 0 \iff \lambda = \pm i$$
$$\Rightarrow \boldsymbol{\left(\vec{\psi}_\lambda^{(j)}\right)^\intercal \vec{\psi}_\lambda^{(j')} = \delta_{jj'} \iff C_\lambda^{(\pm 1)} = \frac{\pm 1}{\sqrt{2(\lambda^2+\sqrt{\lambda^2+1}+1)}}} \quad . \tag{D.9}$$

Moreover, these two eigenvectors possess the following closure property:

$$\boldsymbol{\sum_j \vec{\psi}_\lambda^{(j)} \left(\vec{\psi}_\lambda^{(j)}\right)^\intercal} = \begin{pmatrix} \left(\vec{\psi}_{\lambda,1}^{(1)}\right)^2 + \left(\vec{\psi}_{\lambda,1}^{(-1)}\right)^2 & \vec{\psi}_{\lambda,2}^{(1)}\vec{\psi}_{\lambda,1}^{(-1)} + \vec{\psi}_{\lambda,2}^{(-1)}\vec{\psi}_{\lambda,1}^{(1)} \\ \vec{\psi}_{\lambda,1}^{(1)}\vec{\psi}_{\lambda,2}^{(1)} + \vec{\psi}_{\lambda,1}^{(-1)}\vec{\psi}_{\lambda,2}^{(-1)} & \left(\vec{\psi}_{\lambda,1}^{(1)}\right)^2 + \left(\vec{\psi}_{\lambda,1}^{(-1)}\right)^2 \end{pmatrix} =$$
$$= \begin{pmatrix} \left(2C_\lambda^{(1)}\right)^2 \left(\lambda^2+\sqrt{\lambda^2+1}+1\right) \\ C_\lambda^{(1)}\left[\lambda\left(1+\sqrt{\lambda^2+1}\right) - \lambda\left(1+\sqrt{\lambda^2+1}\right)\right] \end{pmatrix}$$
$$\begin{pmatrix} C_\lambda^{(1)}\left[\lambda\left(1+\sqrt{\lambda^2+1}\right) - \lambda\left(1+\sqrt{\lambda^2+1}\right)\right] \\ \left(2C_\lambda^{(1)}\right)^2 \left(\lambda^2+\sqrt{\lambda^2+1}+1\right) \end{pmatrix} = \boldsymbol{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \iff C_\lambda^{(1)} = C_\lambda^{(-1)} \quad .$$
(D.10)

D.2 Exceptional Points

We will now discus the remaining case when

$$\lambda = \pm i \quad . \tag{D.11}$$

Therefore an ***energy degeneracy occurs***:

$$E_\lambda^{(+1)} = E_\lambda^{(-1)} = 0 \quad . \tag{D.12}$$

We can see that the procedure for generating eigenvectors used in the previous section cannot be used in this case, since

$$\lim_{\lambda\to\pm i} C_\lambda^{(\pm 1)} = \lim_{\lambda\to\pm i} \frac{\pm 1}{\sqrt{2(\lambda^2+\sqrt{\lambda^2+1}+1)}} = \pm\infty \quad ; \tag{D.13}$$

and the expressions used for $C_\lambda^{(\pm 1)}$, (D.7)-(D.8), thus become ill defined for $\lambda = \pm i$. The vectors $\vec{\psi}_\lambda^{(\pm 1)}$ become linearly dependent. This indicates an extremely unusual situation: For $\lambda = \lambda_{\rm EP} = \pm i$, the eigenproblem (D.2) gives rise just to a single eigenvector, namely,

$$\vec{\boldsymbol{\psi}}_{\pm i}^{(1)} = \vec{\boldsymbol{\psi}}_{\pm i}^{(-1)} = \begin{pmatrix} \mathbf{1} \\ \pm \boldsymbol{i} \end{pmatrix} \quad ; \tag{D.14}$$

assuming a convenient normalization. We shall thus hereafter write just $\vec{\psi}_{\pm i}$ rather than $\vec{\psi}_{\pm i}^{(\pm 1)}$. In other words, we encounter here not just eigenvalue degeneracy, but also an ***eigenvector degeneracy occurs*** [29]. This is an extremely peculiar situation known in linear algebra.

The single eigenvector (D.14) is self-orthogonal, i.e.

$$\left(\vec{\psi}_{\pm i}\right)^{\intercal} \vec{\psi}_{\pm i} = 1 + i^2 = 0 \quad . \tag{D.15}$$

Further theoretical developments of the properties of the EPs require an adequate formulation of the closure property. Clearly, the above displayed conventional closure formula (D.10) breaks down, since in the EP situation only a single eigenvector of $\underline{\underline{H_\lambda}}$ exists. For the sake of clarity, we shall from now on consider just the case of $\lambda = +i$. In order to build up a closure type relation we need to add another vector $\vec{\phi} \in \mathbb{C}^2$, linearly independent of $\vec{\psi}_{+i}$. This vector will no longer be an eigenvector of $\underline{\underline{H_{+i}}}$. We require that

$$\vec{\psi}_{+i} \vec{\phi}^{\intercal} + \vec{\phi} \left(\vec{\psi}_{+i}\right)^{\intercal} = \hat{I} \tag{D.16}$$

$$\begin{pmatrix} 1 \\ i \end{pmatrix} \begin{pmatrix} \phi_1 & \phi_2 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \begin{pmatrix} 1 & i \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad . \tag{D.17}$$

Therefore,

$$\begin{aligned} 2\phi_1 = 1 \Rightarrow \phi_1 &= \frac{1}{2} \quad ; \\ 2i\phi_2 = 1 \Rightarrow \phi_2 &= \frac{-i}{2} \quad ; \\ i\phi_1 + \phi_2 = 0 \iff \frac{i}{2} &- \frac{i}{2} = 0 \quad ; \\ \Rightarrow \vec{\boldsymbol{\phi}} &= \frac{\mathbf{1}}{\mathbf{2}} \begin{pmatrix} \mathbf{1} \\ \boldsymbol{-i} \end{pmatrix} \quad . \end{aligned} \tag{D.18}$$

As we can see $\vec{\phi}$ is determined uniquely. The vector $\vec{\psi}_i$ can be obtained from $\vec{\phi}$ thanks to their following important property:

$$\underline{\underline{H_{+i}}} \vec{\phi} = \frac{1}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} 1 \\ i \end{pmatrix} = \vec{\psi}_{+i} \quad . \tag{D.19}$$

This is a very important lemma used frequently in further mathematical developments of the theory of EPs.