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**BACHELOR THESIS**

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**Study of resonance and threshold effects on  
simple two-channel model**

Institute of Theoretical Physics

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Název práce: Studium rezonančních a prahových jevů na jednoduchém dvoukanálovém modelu

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Abstrakt: Táto práca sa venuje jednoduchému jednorozmernému dvojkanálovému rozptylovému modelu, kde bodová interakcia medzi kanálmi je sprostredkovaná delta potenciálom. Tento rozptylový problém je analyticky riešiteľný. Riešením Lippmannovej-Schwingerovej rovnice sú nájdené rozptylové vlastné stavy, následne maticové elementy  $S$  matice a vlastné fázy. Skúma sa vplyv parametrov na prahové a rezonančné javy (prítomnosť, poloha, šírka) a ich vzťah ku pólom  $S$  matice v komplexnej  $k$ -rovine. Potom pre model v rezonančnom režime je aplikovaný projekčný formalizmus a rozptylová  $T$  matica sa separuje na ortogonálny, priamy a rezonančný člen. Diskutuje sa vplyv výberu podpriestoru kvázi-väzbových stavov na separáciu  $T$  matice.

Klíčová slova: kvantová teória rozptylu, dvoukanálový rozptyl, delta potenciál, rezonance

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Abstract: In this thesis we study simple one-dimensional two-channel scattering model where pointlike coupling between channels is provided by the delta potential. The scattering task can be completely solved analytically. The solution of the Lippmann-Schwinger equation leads to improper scattering eigenvectors, consequently to scattering  $S$  matrix elements and eigenphases. We study how the setting of parameters affects threshold and resonant behaviour (presence, position, width) and the mutual relationship between resonances and poles of the  $S$  matrix in complex  $k$ -plane. Then we apply projection-operator formalism to model with resonance and the on-shell  $T$  matrix is separated into the orthogonal, direct and resonant term. We discuss how choice of subspace of quasi-bound states effects the separation.

Keywords: quantum scattering theory, two-channel scattering, delta potential, resonance

At the beginning of this thesis the topic of the scattering theory was for me freshly new. Therefore I would like to thank to my supervisor Martin Čížek for his patience, help and time spent to guide me through this subject and to overcome obstacles hidden in details.

I would also like to thank to my family and friends for their mental and material support.

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# Introduction

Scattering experiments are useful and essential tool of modern physics. They are used in many fields (e.g. particle, nuclear, atomic or molecular physics) and have found wide range of applications in other disciplines too (e.g. crystallography, nuclear medicine). The common element of scattering experiments is collision of particles. The nature of the collision depends on the energy. The low-energy collision usually leads to only one possible outcome – *single-channel (elastic) scattering*. For higher energies the range of possible outcomes is often more interesting (more complex) and we can get more than one configuration – *multichannel scattering*. Another interesting often observed phenomenon are *resonances* – the rapid and sharp change of scattering quantities (e.g. scattering probability) in small interval of energies (Figure 1). They can be often understood as temporary capture of particle into *quasi-bound state*.

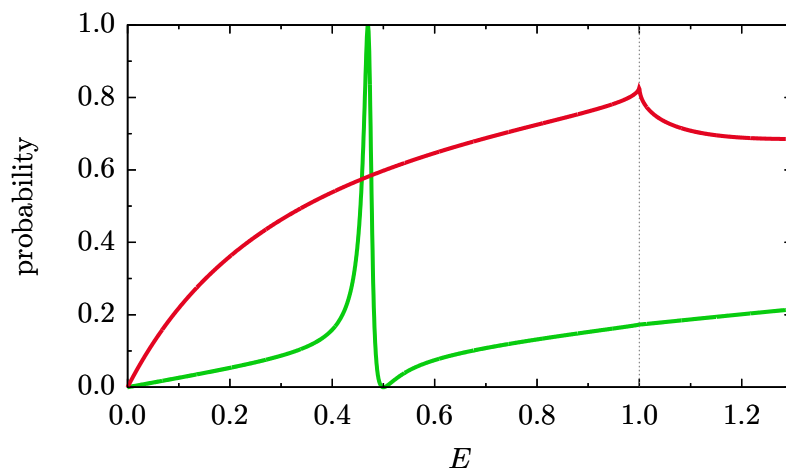
In this thesis we will study simple exactly solvable one-dimensional<sup>1</sup> two-channel scattering model, where we can observe *threshold behaviour* (common in multichannel scattering, Figure 1) and *resonances*. The interaction between two channels is pointlike and is ensured by Dirac delta "function" potential (also called *delta potential*).

The first chapter serves as a short introduction to time-dependent and time-independent formalism of the quantum scattering theory. Bulk of terminology and basic structure is rephrased from or inspired by [6].

The chapter number two is dedicated to same one-dimensional model with delta potential only restricted to one channel. It mainly serves as simpler problem to show instructive application of the framework, but also as reference model without coupling.

The third chapter contains complete solution of the one-dimensional two-channel scattering model and studies influence of parameters on threshold and resonant behaviour. Mutual relation between resonance and poles of the S matrix in complex  $k$ -plane is discussed.

In the fourth chapter we have applied projection-operator formalism to separate background and resonant terms of on-shell T matrix. This separation is commonly used in molecular physics to generalize Born-Oppenheimer approximation for electron-scattering resonance states (e.g. in [1] or [4]). The formalism is outlined in [3] or in [2].



**Figure 1:** The resonant (green line) and threshold (red line) behaviour.

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<sup>1</sup>The scattering in spherical potential can be transformed into one-dimensional scattering.

# 1. The brief introduction to the scattering theory

In this chapter we will make a short introduction to the quantum scattering theory<sup>1</sup>. The terminology, the notation and the basis structure of the scattering theory have been adapted from Taylor's publication [6], where these can be found in more details. In general, the scattering theory is wide framework describing scattering experiments. The *scattering experiment* is (usually a deliberate) collision of (accelerated) particle(s) with a static target (particle(s) with negligible kinetic energy, e.g., atoms) or with another (accelerated) particle(s).

The scattering theory has two main tasks:

1. *Prediction.* The input variables of the experiment (type and kinetic energy of particles, type of target...) are known and can be controlled by experimentalist. The correct scattering theory should provide prediction of probability<sup>2</sup> of certain output variables of the experiment (kinetic energy of outgoing particles, the scattering angle...) or observation of various phenomena (e.g., resonance and threshold effects).
2. *Analysis.* Oppositely to the previous task the output variables of the experiment and the nature of interactions are known (and possibly some input variables). The scattering theory should provide information about ingoing particles or about target (type of particles, kinetic energy...). In general the difficulty of this task depends on amount of known information.

This thesis will be dealing with the first task.

## 1.1 Preliminaries

In formalism of spectral decomposition the eigenvectors of Hermitian operator (or set of operators called *complete set of commuting observables* (CSCO)) form *orthonormal basis* of the corresponding *Hilbert space*  $\mathcal{H}$ . In the scattering theory it is convenient<sup>3</sup> to work with the momentum eigenvectors  $|\mathbf{p}\rangle$ .<sup>4</sup> In position representation they can be expressed as<sup>5,6,7</sup>

$$\langle x|\mathbf{p}\rangle = (2\pi)^{-1/2} e^{i\mathbf{p}x} . \quad (1.1)$$

---

<sup>1</sup>In the whole thesis the scattering is described on the level of the non-relativistic quantum mechanics.

<sup>2</sup>The scattering theory of our interest is based on quantum mechanics, therefore the probabilistic interpretation is in the nature of this theory. We cannot predict results of experiment, we can only determinate the probability for all possible results.

<sup>3</sup>The convenience will arise in the second property of the scattering operator  $\widehat{S}$ .

<sup>4</sup>The vector  $|\mathbf{p}\rangle$  can also be denoted as vector  $|p, \hat{\mathbf{p}}\rangle$  by the magnitude  $p := |\mathbf{p}|$  and unit vector  $\hat{\mathbf{p}} := \frac{\mathbf{p}}{p}$  of momentum vector  $\mathbf{p}$ , specifically in 1D as  $|p, s\rangle$ , where  $s := \text{sgn}(\mathbf{p}) = \pm 1$  is the direction of the momentum.

<sup>5</sup>In our thesis we will be dealing only with one-dimensional scattering, hence everywhere the dimensionality is equal to 1. But whole concept of the scattering theory is independent of dimensionality and can be performed without this specification.

<sup>6</sup>In suitable units we can choose  $\hbar = 1$ .

<sup>7</sup>Even though we work in one dimension, we preserve the vector notation for momentum to make difference between the momentum  $\mathbf{p}$  (real number) and the magnitude of the momentum  $p$  (non-negative number).

The momentum eigenvectors  $|\mathbf{p}\rangle$  are *improper vectors* (non-square-integrable).<sup>8</sup>

If some operator  $\widehat{B} := f(\widehat{A})$  is defined as some function<sup>9</sup> of the other operator, they have same eigenvectors

$$\widehat{A}|n\rangle = a_n|n\rangle \implies \widehat{B}|n\rangle = f(a_n)|n\rangle. \quad (1.2)$$

## 1.2 Time-dependent scattering theory

Typically a single scattering experiment can be roughly divided into three phases:

1. several particles are in large separation from each other (so they don't interact with each other) approaching on collision course,
2. collision and interaction of particles,
3. particles flying away to large separation from each other.

To define more precisely the basic terminology of the scattering theory we will choose the simplest scattering experiment: the scattering of a single spinless particle by fixed potential (e.g., the potential of atom) also known as *potential scattering*.<sup>10,11</sup> We assume time-independent Hamiltonian of single particle  $\widehat{H}(t) = \widehat{H}$

$$\widehat{H} = \widehat{T} + \widehat{V},$$

where  $\widehat{T}$  is operator of kinetic energy and  $\widehat{V}$  operator of potential energy. The system at the instant  $t$  is described by a state vector  $|\psi(t)\rangle$ , which satisfies the *time-dependent Schrödinger equation* with the formal solution

$$i \frac{d}{dt} |\psi(t)\rangle = \widehat{H} |\psi(t)\rangle \implies |\psi(t)\rangle = \underbrace{e^{-i\widehat{H}t}}_{=: \widehat{U}(t)} |\psi\rangle, \quad (1.3)$$

where  $\widehat{U}(t)$  is the *evolution operator* and  $|\psi\rangle$  has meaning of the state vector at the time  $t = 0$  ( $|\psi(0)\rangle = |\psi\rangle \in \mathcal{H}$ ).<sup>12</sup>

The Hamiltonian  $\widehat{H}$  can be divided into Hamiltonian of free particle  $\widehat{H}_0$  (the *free Hamiltonian*) and the interaction potential  $\widehat{V}$

$$\widehat{H} = \underbrace{\widehat{T}}_{=: \widehat{H}_0} + \widehat{V}. \quad (1.4)$$

In the infinite time limit  $t \rightarrow \pm\infty$  (both before and after the collision) the motion of the particle is determined by free Hamiltonian  $\widehat{H}_0$  and there exist incoming ( $|\psi_{\text{in}}\rangle$ ) and outgoing ( $|\psi_{\text{out}}\rangle$ ) particle asymptotes.<sup>13</sup>

<sup>8</sup>The handling of improper vectors is same as of proper vectors, but every mathematical treatment must be underpinned by rigorous justification. In general, we will treat them same and we will note every difference from proper vectors if such occurs. Especially in scattering theory there are statements which hold for any square-integrable vector, but are false for improper vectors.

<sup>9</sup>We can define the operator  $\widehat{B}$  other way around on eigenvectors of the operator  $\widehat{A}$ . Then the only condition for the function  $f$  is to be defined on eigenvalues  $a_n$ .

<sup>10</sup>Since the elastic scattering of two particles described in their center-of-mass frame of reference is equivalent to the scattering of a single particle by a fixed potential, this scattering problem is also important in two-particle scattering theory.

<sup>11</sup>The terminology can be generalised for more complicated systems. Our objective is to become familiar with terminology using also intuition based on classical mechanics.

<sup>12</sup>When we talk about real physical states of scattering particle, we will think of them as wave packets.

<sup>13</sup>This is not true for any arbitrary potential. Mathematics: The potential  $\widehat{V}$  must satisfy conditions, which ensure the existence of the infinite time limit. Physics: When the particle (wave packet) is localised in large distance from target atom, the potential vanishes and does not affect the particle.



The motion of free particle is described by a state vector  $|\psi_{\text{in/out}}(t)\rangle$ , which satisfies the time-dependent Schrödinger equation with the formal solution

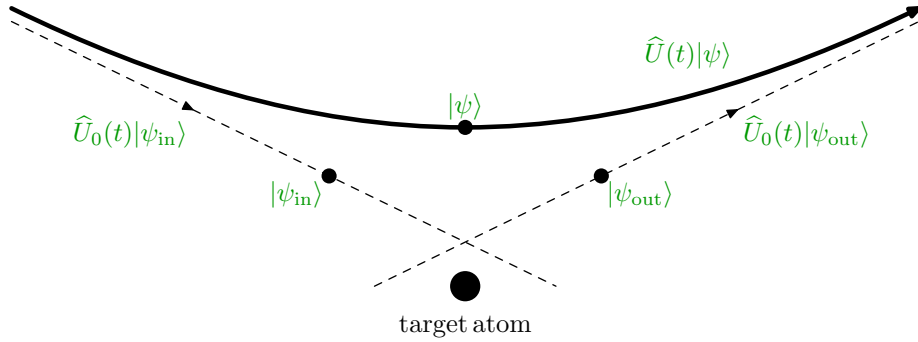
$$i \frac{d}{dt} |\psi_{\text{in/out}}(t)\rangle = \widehat{H}_0 |\psi_{\text{in/out}}(t)\rangle \implies |\psi_{\text{in/out}}(t)\rangle = \underbrace{e^{-i\widehat{H}_0 t}}_{=: \widehat{U}_0(t)} |\psi_{\text{in/out}}\rangle, \quad (1.5)$$

where  $\widehat{U}_0(t)$  is the *free evolution operator* and  $|\psi_{\text{in/out}}\rangle$  has analogous meaning as before in equation (1.3).

Mathematically, the incoming/outgoing asymptote  $|\psi_{\text{in/out}}(t)\rangle$  approaches the state evolution  $|\psi(t)\rangle$  in the limit<sup>14</sup>

$$\lim_{t \rightarrow \mp\infty} \|\psi_{\text{in/out}}(t) - \psi(t)\| = 0. \quad (1.6)$$

This concept can be illustrated schematically as shown in Figure 1.1.<sup>15</sup>



**Figure 1.1:** The asymptotes  $|\psi_{\text{in/out}}(t)\rangle$  of the orbit  $|\psi(t)\rangle$  in the scattering of a single spinless particle by fixed atom.

The interaction time in scattering experiment is usually short ( $\approx 10^{-10}$  s), thus we can only measure the free motion of particles before and after collision ( $|\psi_{\text{in}}(t)\rangle$  and  $|\psi_{\text{out}}(t)\rangle$ ). Therefore the basic task of scattering theory is to determine relationship between states  $|\psi_{\text{in}}\rangle$  and  $|\psi_{\text{out}}\rangle$ .<sup>16</sup> This relation is given by the *scattering operator*  $\widehat{S}$ . From condition (1.6) it also follows that the state  $|\psi\rangle$  is linearly related to states  $|\psi_{\text{in/out}}\rangle$  by operators called the *Møller operators*  $\widehat{\Omega}_{\pm}$ .

$$\begin{aligned} \widehat{S} : \mathcal{H} &\rightarrow \mathcal{H} & \widehat{\Omega}_+ : \mathcal{H} &\rightarrow \mathcal{H} & \widehat{\Omega}_- : \mathcal{H} &\rightarrow \mathcal{H} \\ |\psi_{\text{in}}\rangle &\rightarrow |\psi_{\text{out}}\rangle & |\psi_{\text{in}}\rangle &\rightarrow |\psi\rangle & |\psi_{\text{out}}\rangle &\rightarrow |\psi\rangle \end{aligned}$$

We can "move" along the dashed lines and bold line in Figure 1.1 by acting the free evolution operator  $\widehat{U}_0(t)$  and the evolution operator  $\widehat{U}(t)$  respectively. Hence we can properly define the Møller operators  $\widehat{\Omega}_{\pm}$  and the scattering operator  $\widehat{S}$  using the evolution operators as shown in Figure 1.2 as<sup>17</sup>

$$\widehat{\Omega}_{\pm} := \lim_{t \rightarrow \mp\infty} \widehat{U}(t)^+ \widehat{U}_0(t) \quad \widehat{S} := \widehat{\Omega}_-^+ \widehat{\Omega}_+. \quad (1.7)$$

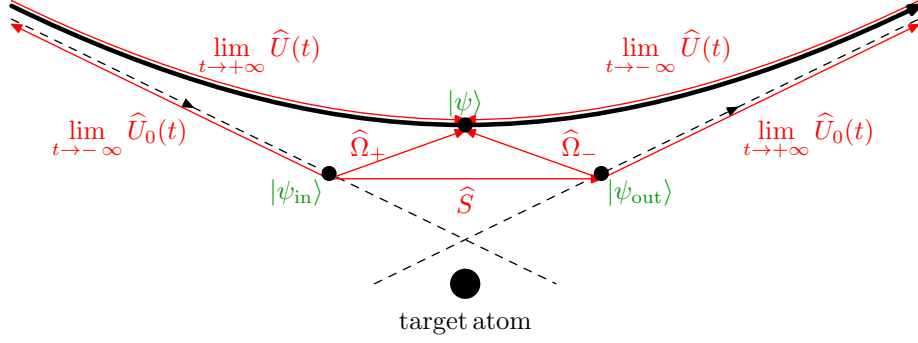
The properties of the Møller operators:

<sup>14</sup>As already pointed out, the existence of the limit depends on the potential  $\widehat{V}$ . For not fast enough decreasing potential (e.g. Coulomb potential) the limit does not exist. For potential satisfying so called *the asymptotic condition(s)* there exists the limit for any state vector  $|\psi\rangle \in \mathcal{H}$ .

<sup>15</sup>The figure can be understood in terms of *classic mechanics* [*quantum mechanics*] as an *orbit* of pointlike particle  $\mathbf{r}(t)$  [ $\widehat{U}(t)|\psi\rangle$ ] with asymptotic orbits  $\mathbf{r}_{\text{in/out}}(t)$  [ $\widehat{U}_0(t)|\psi_{\text{in/out}}\rangle$ ] – straight dashed lines – in real space  $\mathbb{R}^3$  [Hilbert space  $\mathcal{H}$ ] with a marked positions  $\mathbf{r}(0)$ ,  $\mathbf{r}_{\text{in/out}}(0)$  [states  $|\psi\rangle$ ,  $|\psi_{\text{in/out}}\rangle$ ] in certain instant.

<sup>16</sup>One could argue that the whole free motion is described by whole orbits  $|\psi_{\text{in}}(t)\rangle$  and  $|\psi_{\text{out}}(t)\rangle$ , not by states  $|\psi_{\text{in}}\rangle$  and  $|\psi_{\text{out}}\rangle$ . But the orbits are uniquely determined via formula (1.5) thus our approach is valid.

<sup>17</sup>It is convenient to note  $\widehat{U}(t)^+ = \widehat{U}(-t)$ .



**Figure 1.2:** Definition of the Møller operators  $\hat{\Omega}_{\pm}$  and the scattering operator  $\hat{S}$ .

1. *Orthogonality theorem.* For potential  $\hat{V}$  satisfying the asymptotic condition:  $\mathcal{R}_+ \perp \mathcal{B}$  and  $\mathcal{R}_- \perp \mathcal{B}$ . (We denote  $\mathcal{R}_{\pm}$  as the range of the Møller operator  $\hat{\Omega}_{\pm}$  and  $\mathcal{B}$  as subspace of bound states.)
2. *Asymptotic completeness.* If  $\mathcal{R}_+ = \mathcal{R}_- =: \mathcal{R}$ , then the scattering theory is called asymptotically complete.<sup>18</sup> The Møller operators map from space  $\mathcal{H}$  (space of asymptotes) onto the subspace  $\mathcal{R}$  (space of scattering states).

$$\underbrace{|\psi\rangle}_{\in \mathcal{R}} = \hat{\Omega}_+ \underbrace{|\psi_{\text{in}}\rangle}_{\in \mathcal{H}} = \hat{\Omega}_- \underbrace{|\psi_{\text{out}}\rangle}_{\in \mathcal{H}} \quad (1.8)$$

3. *Isometry.* The Møller operators are defined as limit of product of unitary operators, consequently they preserve the norm. But unlike the unitary operator<sup>19</sup> (which maps  $\mathcal{H}$  onto  $\mathcal{H}$ ) the Møller operators maps  $\mathcal{H}$  onto  $\mathcal{R}$ . Therefore

$$\hat{\Omega}_{\pm}^{\dagger} \hat{\Omega}_{\pm} = \hat{1}_{\mathcal{H}}, \quad \hat{\Omega}_{\pm} \hat{\Omega}_{\pm}^{\dagger} = \hat{1}_{\mathcal{R}}.$$

which implies isometry on  $\mathcal{H}$  (and unitarity on  $\mathcal{R}$ ).<sup>20</sup>

4. *Intertwining relation.*<sup>21</sup>

$$\hat{H} \hat{\Omega}_{\pm} = \hat{\Omega}_{\pm} \hat{H}_0 \quad (1.9)$$

The properties of the scattering operator  $\hat{S}$ :

1. *Unitarity.* The scattering operator is unitary operator. This follows directly from definition (1.7) and asymptotic completeness (1.8).<sup>22</sup>

$$\hat{S}^{\dagger} \hat{S} = \hat{S} \hat{S}^{\dagger} = \hat{1}$$

2. *Eigenvalues.* Eigenvalues of the scattering operator  $\hat{S}$  lie on the unit circle:<sup>23</sup>

$$\hat{S} |\psi_{s_n}\rangle = s_n |\psi_{s_n}\rangle \implies |s_n| = 1 \quad s_n =: e^{2i\delta_n}, \quad \delta_n \in \mathbb{R},$$

<sup>18</sup>This directly implies that Hilbert space can be written as the direct sum:  $\mathcal{H} = \mathcal{R} \oplus \mathcal{B}$ .

<sup>19</sup>Unitarity:  $\hat{U}^{\dagger} \hat{U} = \hat{U} \hat{U}^{\dagger} = \hat{1}$ .

<sup>20</sup>The operators  $\hat{\Omega}_{\pm}^{\dagger}$  have similar (but not the same) property called *coisometry* on  $\mathcal{H}$  (preserving the norm, mapping from  $\mathcal{R}$  to  $\mathcal{H}$ ).

<sup>21</sup>The result can be proved in 3 steps: proving expression  $e^{i\hat{H}t} \hat{\Omega}_{\pm} = \hat{\Omega}_{\pm} e^{i\hat{H}_0 t}$  from definition of the Møller operators (1.7), Taylor expansion of previous expression at  $t = 0$  and comparison of both sides term by term.

<sup>22</sup>The operator  $\hat{\Omega}_+$  is isometric operator from  $\mathcal{H}$  onto  $\mathcal{R}$ , the operator  $\hat{\Omega}_-^{\dagger}$  is coisometric operator from  $\mathcal{R}$  onto  $\mathcal{H}$ , so their composition is unitary operator from  $\mathcal{H}$  onto  $\mathcal{H}$ .

<sup>23</sup>This is property of any unitary operator.

$$\langle \psi_{s_n} | \psi_{s_n} \rangle = \langle \psi_{s_n} | \hat{1} | \psi_{s_n} \rangle = \langle \psi_{s_n} | \hat{S}^{\dagger} \hat{S} | \psi_{s_n} \rangle = s_n^* s_n \langle \psi_{s_n} | \psi_{s_n} \rangle \implies |s_n| = 1,$$

where eigenvectors have non-zero norm (eigenvectors cannot be zero vector).

where we can define real-valued quantity  $\delta_n$  called *eigenphase* or *phase shift*. There is ambiguity in the definition of phase shift  $\delta_n$  up to additional multiple of  $\pi$ . The factor 2 is added for quantity  $\delta_n$  to represent conventional phase shift.<sup>24</sup>

### 3. Conservation of energy.<sup>25</sup>

$$\widehat{S}^+ \widehat{H}_0 \widehat{S} = \widehat{H}_0 \xleftrightarrow[\widehat{S}^+]{\widehat{S}} [\widehat{S}, \widehat{H}_0] = 0 \quad (1.10)$$

This relation can be understood as follows: Energy measured on incoming ( $|\psi_{\text{in}}\rangle$ ) and outgoing ( $|\psi_{\text{out}}\rangle$ ) asymptote is equal (we measure energy with free Hamiltonian  $\widehat{H}_0$ ).

$$E_{\text{in}} := \langle \psi_{\text{in}} | \widehat{H}_0 | \psi_{\text{in}} \rangle = \langle \psi_{\text{in}} | \widehat{S}^+ \widehat{H}_0 \widehat{S} | \psi_{\text{in}} \rangle \xrightarrow{|\psi_{\text{out}}\rangle = \widehat{S} |\psi_{\text{in}}\rangle} \langle \psi_{\text{out}} | \widehat{H}_0 | \psi_{\text{out}} \rangle =: E_{\text{out}}$$

It is convenient due to commutation relation (1.10) to choose the eigenvectors of the free Hamiltonian  $\widehat{H}_0$  for the orthonormal basis. Equation (1.2) for free Hamiltonian  $\widehat{H}_0 = \frac{\widehat{p}^2}{2}$  implies that

$$\widehat{H}_0 |\mathbf{p}\rangle = \underbrace{\frac{p^2}{2}}_{=: E_p} |\mathbf{p}\rangle. \quad (1.11)$$

### 4. Matrix elements.<sup>26</sup> From matrix elements of (1.10) it follows that

$$0 = \langle \mathbf{p}' | [\widehat{S}, \widehat{H}_0] | \mathbf{p} \rangle = (E_{p'} - E_p) \langle \mathbf{p}' | \widehat{S} | \mathbf{p} \rangle,$$

which implies that the matrix element  $\langle \mathbf{p}' | \widehat{S} | \mathbf{p} \rangle$  is zero for  $E_{p'} \neq E_p$  and can be written as<sup>27</sup>

$$\langle \mathbf{p}' | \widehat{S} | \mathbf{p} \rangle = \delta(E_{p'} - E_p) \times \text{remainder}. \quad (1.12)$$

With no scattering potential ( $\widehat{H} = \widehat{H}_0$ ) the scattering operator is pure identity operator  $\widehat{S} = \widehat{1}$ , hence it is useful to look at the scattering operator in the form  $\widehat{S} = \widehat{1} + \widehat{R}$ , which can be written with respect to (1.12) as<sup>28</sup>

$$\langle \mathbf{p}' | \widehat{S} | \mathbf{p} \rangle = \delta(\mathbf{p}' - \mathbf{p}) - 2\pi i \delta(E_{p'} - E_p) t(\mathbf{p}' \leftarrow \mathbf{p}), \quad (1.13)$$

where we have defined the *on-shell T matrix*  $t(\mathbf{p}' \leftarrow \mathbf{p})$ .<sup>29</sup>

<sup>24</sup>It can be shown, that the free asymptotic solution  $\langle x | \psi_{\text{in/out}} \rangle$  and the full solution  $\langle x | \psi \rangle$  synchronised at the origin  $x = 0$  are in the limit  $x \rightarrow \pm\infty$  shifted by *phase shift*  $\delta_n$ . This is the origin of the term.

<sup>25</sup>This can be proved using the intertwining relation (1.9).

$$\widehat{S} \widehat{H}_0 = \widehat{\Omega}_+^+ \widehat{\Omega}_+ \widehat{H}_0 \stackrel{(1.9)}{=} \widehat{\Omega}_+^+ \widehat{H} \widehat{\Omega}_+ = (\widehat{H} \widehat{\Omega}_-)^+ \widehat{\Omega}_+ \stackrel{(1.9)}{=} (\widehat{\Omega}_- \widehat{H}_0)^+ \widehat{\Omega}_+ = \widehat{H}_0 \widehat{\Omega}_+^+ \widehat{\Omega}_+ = \widehat{H}_0 \widehat{S}$$

<sup>26</sup>When we talk about matrix elements  $\langle \mathbf{p}' | \widehat{S} | \mathbf{p} \rangle$  and processes with incoming ( $\mathbf{p}$ ) and outgoing ( $\mathbf{p}'$ ) momentum, the vectors  $|\mathbf{p}\rangle$  are improper (so they do not represent any physical state), but we can imagine sequence of wave packets  $\langle \mathbf{p} | \psi_j \rangle$  with mean momentum  $\mathbf{p}$  and gradually smaller and smaller variance in momentum space.

<sup>27</sup>This relation expresses the conservation of energy before and after the scattering experiment.

<sup>28</sup>The arbitrary prefactor  $-2\pi i$  is chosen for later convenience.

<sup>29</sup>The term "on-shell" means that it is defined only on the energy shell  $E_{p'}$ , only for momenta  $\mathbf{p}'$  and  $\mathbf{p}$  which correspond to same energy  $E_{p'} = E_p$  because of the term  $\delta(E_{p'} - E_p)$ . Based on this definition it would make no sense to talk about values of T matrix for  $\mathbf{p}'$  and  $\mathbf{p}$ , where  $E_{p'} \neq E_p$ . Later on we will define  $\widehat{T}$  operator whose matrix elements  $\langle \mathbf{p}' | \widehat{T} | \mathbf{p} \rangle$  will be naturally defined for every momenta  $\mathbf{p}'$  and  $\mathbf{p}$  and it will coincide with the on-shell T matrix elements.

### 1.3 Time-independent scattering theory

Up to now we have discussed scattering theory based on the terminology of the time evolution operators  $\widehat{U}(t)$  and  $\widehat{U}_0(t)$  and derived operators ( $\widehat{\Omega}_\pm$ ,  $\widehat{S}$  and  $t(\mathbf{p}' \leftarrow \mathbf{p})$ ). The direct calculation from definitions for given system is impractical for analytic calculation. But there is approach which provides time-independent framework which is more convenient for practical calculation.

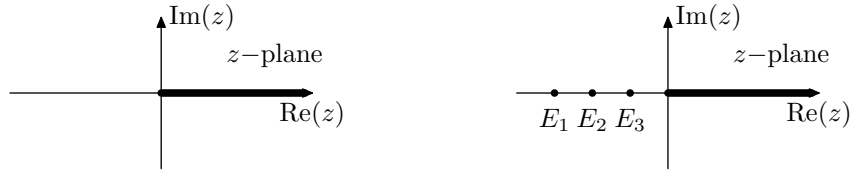
The useful tool to define for algebraic formulation of the scattering quantities is *Green's operator* (in mathematics often called *resolvent*). The Green's operator  $\widehat{G}(z)$  and the free Green's operator  $\widehat{G}_0(z)$  are defined as

$$\widehat{G}(z) := (z - \widehat{H})^{-1}, \quad \widehat{G}_0(z) := (z - \widehat{H}_0)^{-1} \quad (1.14)$$

for any complex  $z$ , if the inverse exists.<sup>30</sup> According to spectral decomposition the set of eigenvectors of the (free) Hamiltonian  $\widehat{H}$  ( $\widehat{H}_0$ ) can form orthogonal basis  $\{|E, \alpha\rangle\}$ <sup>31</sup>, thus using (1.2) the (free) Green's operator  $\widehat{G}(z)$  ( $\widehat{G}_0(z)$ ) can be expressed as

$$\widehat{G}(z) = \sum_{\alpha} \prod_E dE \frac{|E, \alpha\rangle\langle E, \alpha|}{z - E}. \quad (1.15)$$

Therefore we can see, that Green's operators  $\widehat{G}(z)$  and  $\widehat{G}_0(z)$  are well-defined and analytic operator<sup>32</sup> everywhere except for  $z$  equal to eigenvalues (Figure 1.3).



**Figure 1.3:** Analyticity of the free Green's operator  $\widehat{G}_0(z)$  (left) and the Green's operator  $\widehat{G}(z)$  (right) in  $z$ -plane.

For operator  $\widehat{G}(z)$  there are isolated poles ( $E < 0$ , the bound states) and continuous cut from 0 to  $+\infty$  ( $E > 0$ , the scattering states). The operator  $\widehat{G}_0(z)$  is analytic for every  $z$  except for continuous cut from 0 to  $+\infty$ .

Because of the relation between the Hamiltonian  $\widehat{H}$  and the free Hamiltonian  $\widehat{H}_0$

$$\widehat{H} = \widehat{H}_0 + \widehat{V}$$

the Green's operators  $\widehat{G}(z)$  and  $\widehat{G}_0(z)$  are intertwined. From definitions (1.14) we obtain

$$\widehat{G}_0(z)^{-1} = \widehat{G}(z)^{-1} + \widehat{V}.$$

In order to get rid of the inverses we will act with operator  $\widehat{G}_0(z)$  on the left [right] and  $\widehat{G}(z)$  on the right [left] and we will gain operator relation(s) relating operators  $\widehat{G}(z)$  and  $\widehat{G}_0(z)$  called *Lippmann-Schwinger equation for  $\widehat{G}(z)$* .

$$\widehat{G}(z) = \widehat{G}_0(z) + \widehat{G}_0(z)\widehat{V}\widehat{G}(z), \quad \widehat{G}(z) = \widehat{G}_0(z) + \widehat{G}(z)\widehat{V}\widehat{G}_0(z). \quad (1.16)$$

<sup>30</sup>We allow complex values of  $z$ , because it turns out that *the complex analysis* is useful tool of modern scattering theory.

<sup>31</sup>For instance, in 3D the CSCO  $\{\widehat{H}_0, \widehat{L}^2, \widehat{L}_z\}$  forms orthonormal basis  $\{|E, l, m\rangle\}$ .

<sup>32</sup>The operator is analytic, when for any 2 state vectors the matrix element  $\langle\phi|\widehat{G}(z)|\psi\rangle$  is analytic function of the complex variable  $z$ .

We introduce the operator  $\widehat{T}(z)$ <sup>33</sup>

$$\widehat{T}(z) := \widehat{V} + \widehat{V}\widehat{G}(z)\widehat{V}. \quad (1.17)$$

From definition it is clear that the operator  $\widehat{T}(z)$  has the same analyticity as the operator  $\widehat{G}(z)$ . From definition (1.17) and (1.16) we get operator identities

$$\widehat{G}_0(z)\widehat{T}(z) = \widehat{G}(z)\widehat{V}, \quad \widehat{T}(z)\widehat{G}_0(z) = \widehat{V}\widehat{G}(z), \quad (1.18)$$

and from the first identity and definition (1.17) we obtain *Lippmann-Schwinger equation* for  $\widehat{T}(z)$ <sup>34</sup>

$$\widehat{T}(z) = \widehat{V} + \widehat{V}\widehat{G}_0(z)\widehat{T}(z).$$

In the following lines we will attempt to develop time-independent scattering theory for basic terms in time-dependent theory. We will begin with the Møller operators  $\widehat{\Omega}_\pm$

$$\widehat{\Omega}_\pm|\psi\rangle = \lim_{t \rightarrow \mp\infty} \widehat{U}(t)^+ \widehat{U}_0(t)|\psi\rangle$$

and operator identity (for continuously differentiable operator  $\widehat{A}(t)$ )

$$\widehat{A}(t) = \widehat{A}(0) + \int_0^t d\tau \frac{d\widehat{A}}{d\tau}(\tau).$$

For the operator  $\widehat{A}(t) = \widehat{U}(t)^+ \widehat{U}_0(t)$  we get<sup>35</sup>

$$\widehat{A}(0) = e^{i\widehat{H}_0} e^{-i\widehat{H}_0} = \widehat{1}, \quad \frac{d\widehat{A}}{dt}(t) = \frac{d}{dt} \left( e^{i\widehat{H}t} e^{-i\widehat{H}_0 t} \right) = i\widehat{U}(t)^+ \widehat{V} \widehat{U}_0(t).$$

---

<sup>33</sup>From analogy of pairs  $\widehat{H}$  and  $\widehat{H}_0$ ,  $\widehat{G}(z)$  and  $\widehat{G}_0(z) \dots$ , it would be natural to define the free operator  $\widehat{T}_0(z)$ , but it is clear that would be pure zero operator  $\widehat{0}$ . Similarly, the free scattering operator  $\widehat{S}_0$  would be the unit operator  $\widehat{1}$ .

<sup>34</sup>This equation is more useful than definition, because we usually do not know matrix elements of the Green's operator  $\widehat{G}(z)$  for certain Hamiltonian, but we do know matrix elements of the free Green's operator  $\widehat{G}_0(z)$  (more appendix A.1).

<sup>35</sup>It is instructive to recall

$$\widehat{U}(t) = e^{-i\widehat{H}t}, \quad \widehat{U}(t)^+ = e^{i\widehat{H}t}, \quad \widehat{U}_0(t) = e^{-i\widehat{H}_0 t}, \quad \widehat{U}_0(t)^+ = e^{i\widehat{H}_0 t}.$$

leading to<sup>36</sup>

$$\underbrace{\widehat{\Omega}_{\pm}|\psi\rangle}_{=:\psi_{\pm}} = |\psi\rangle + i \lim_{t \rightarrow \mp\infty} \int_0^t \underbrace{d\tau \widehat{U}(\tau)^{\dagger} \widehat{V} \widehat{U}_0(\tau) |\psi\rangle}_{=:\chi(\tau)} \overbrace{=}^{=:\phi(t)}$$

Now we will use trick and introduce so called *dumping factor*<sup>38</sup>

$$\int_0^{\mp\infty} d\tau |\chi(\tau)\rangle = \lim_{\varepsilon \rightarrow \mp 0} \int_0^{\mp\infty} d\tau e^{-\varepsilon\tau} |\chi(\tau)\rangle.$$

Using furthermore the momentum expansion of the state vector  $|\psi\rangle$ <sup>39</sup>

$$\begin{aligned} |\psi_{\pm}\rangle &= |\psi\rangle + i \lim_{\varepsilon \rightarrow \mp 0} \int_{\mathbb{R}} d\mathbf{p} \underbrace{\int_0^{\mp\infty} d\tau e^{(-\varepsilon - iE_p + i\widehat{H})\tau} \widehat{V} |\mathbf{p}\rangle \psi(\mathbf{p})}_{\text{underwaved}} \\ &= |\psi\rangle + \int_{\mathbb{R}} d\mathbf{p} \widehat{G}(E_p \pm i0) \widehat{V} |\mathbf{p}\rangle \psi(\mathbf{p}). \end{aligned} \quad (1.20)$$

<sup>36</sup>Justification of the existence of the limit: The existence of the limit is equivalent to convergence of the integral as the sequence  $|\phi(t)\rangle$  in  $\mp\infty$ , in the Hilbert space equivalent to *Cauchy convergence condition*

$$\|\phi(t) - \phi(t')\| \xrightarrow{t, t' \rightarrow \mp\infty} 0 \iff \left\| \int_t^{t'} d\tau |\chi(\tau)\rangle \right\| \xrightarrow{t, t' \rightarrow \mp\infty} 0.$$

The stronger condition (from triangular inequality) is  $\int_t^{t'} d\tau \|\chi(\tau)\| \xrightarrow{t, t' \rightarrow \mp\infty} 0$ , which is Cauchy condition for Cauchy sequence  $\int_0^t d\tau \|\chi(\tau)\|$  in the space of real numbers  $\mathbb{R}$  (also Hilbert space with multiplication as the inner product). As we have mentioned a moment ago, this is equivalent to the convergence of  $\int_0^{\mp\infty} d\tau \|\chi(\tau)\| < \infty$ . We retrieve  $|\chi(\tau)\rangle$

$$\int_0^{\mp\infty} d\tau \|\widehat{U}(\tau)^{\dagger} \widehat{V} \widehat{U}_0(\tau) \psi\| = \int_0^{\mp\infty} d\tau \|\widehat{V} \widehat{U}_0(\tau) \psi\| < \infty$$

and for Gaussian function<sup>37</sup>  $\langle x|\psi(x_0, \sigma)\rangle = \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$  we obtain

$$\mp \int_0^{\mp\infty} d\tau \|\widehat{V} \widehat{U}_0(\tau) \psi\| \leq 2.622\sigma^2 \left( \int_{\mathbb{R}} dx |V(x)|^2 \right)^{1/2} < +\infty \implies \int_{\mathbb{R}} dx |V(x)|^2 < +\infty.$$

This is only the necessary condition for the potential (we have used some inequalities). The sufficient condition (called *asymptotic condition*) is weaker. We assume that, this condition is fulfilled and consequently the limit exists.

<sup>37</sup>It is important to highlight this: If the sequence is convergent for Gaussian function, it is also convergent for any finite linear combination of Gaussian functions. And any function of  $\mathcal{L}^2(\mathbb{R}^N)$  can be replaced by finite linear combination of Gaussian functions with arbitrary accuracy.

<sup>38</sup>Justification of dumping factor: We proved convergence and absolute convergence of the integral  $\int_0^{\mp\infty} d\tau |\chi(\tau)\rangle$ . Due to *Lebesgue's dominated convergence theorem*, it is allowed to interchange limit and integration if there exists dominating integrable function. The function  $\|\chi(\tau)\|$  is integrable (absolute convergence) and dominating

$$1 \|\chi(\tau)\| \geq e^{-\varepsilon\tau} \|\chi(\tau)\| = \|e^{-\varepsilon\tau} \chi(\tau)\|,$$

therefore interchange is justified

$$\lim_{\varepsilon \rightarrow \mp 0} \int_0^{\mp\infty} d\tau e^{-\varepsilon\tau} |\chi(\tau)\rangle = \int_0^{\mp\infty} d\tau \lim_{\varepsilon \rightarrow \mp 0} e^{-\varepsilon\tau} |\chi(\tau)\rangle = \int_0^{\mp\infty} d\tau |\chi(\tau)\rangle.$$

<sup>39</sup>The underwaved was evaluated as

$$\int_0^{\mp\infty} d\tau e^{(-\varepsilon - iE_p + i\widehat{H})\tau} = \left[ \frac{e^{(-\varepsilon - iE_p + i\widehat{H})\tau}}{(-\varepsilon - iE_p + i\widehat{H})} \right]_0^{\mp\infty} \stackrel{(1.14)}{=} \frac{1}{z = E_p - i\varepsilon} = -i\widehat{G}(E_p - i\varepsilon). \quad (1.19)$$

Without the dumping factor, we would get stuck on two spots: evaluation of under-waved integral (1.19) (the upper limit does not vanishes, it oscillates) and analyticity of the free Green's operator (Figure 1.3, it is not defined for  $E_p \geq 0$ ). Hence introduction of the dumping factor was inevitable and at the same time rigorous.

We denote (as for proper vectors  $|\psi\rangle$ ) two improper vectors<sup>40</sup>

$$|\mathbf{p}\pm\rangle := \widehat{\Omega}_\pm|\mathbf{p}\rangle,$$

which coincidentally are eigenvectors of the Hamiltonian  $\widehat{H}$  (the scattering states)

$$\widehat{H}|\mathbf{p}\pm\rangle = \widehat{H}\widehat{\Omega}_\pm|\mathbf{p}\rangle \stackrel{(1.9)}{=} \widehat{\Omega}_\pm\widehat{H}_0|\mathbf{p}\rangle = E_p\widehat{\Omega}_\pm|\mathbf{p}\rangle = E_p|\mathbf{p}\pm\rangle.$$

From (1.20) we conclude

$$|\mathbf{p}\pm\rangle = |\mathbf{p}\rangle + \widehat{G}(E_p \pm i0)\widehat{V}|\mathbf{p}\rangle. \quad (1.21)$$

Using the same technique for the scattering operator<sup>41</sup>  $\widehat{S}$  we get for matrix elements  $\langle\mathbf{p}'|\widehat{S}|\mathbf{p}\rangle$

$$\langle\mathbf{p}'|\widehat{S}|\mathbf{p}\rangle = \delta(\mathbf{p}' - \mathbf{p}) - 2\pi i\delta(E_{p'} - E_p) \underbrace{\langle\mathbf{p}'|\widehat{T}(E_p + i0)|\mathbf{p}\rangle}_{t(\mathbf{p}' \leftarrow \mathbf{p})}, \quad (1.22)$$

which link relationship between the operator  $\widehat{T}(z)$  and the on-shell T matrix  $t(\mathbf{p}' \leftarrow \mathbf{p})$ .

From definition (1.17) we obtain

$$\widehat{T}(E_p \pm i0)|\mathbf{p}\rangle \stackrel{(1.17)}{=} \widehat{V} \left[ \widehat{1} + \widehat{G}(E_p \pm i0)\widehat{V} \right] |\mathbf{p}\rangle \stackrel{(1.21)}{=} \widehat{V}|\mathbf{p}\pm\rangle. \quad (1.23)$$

This leads to two convenient<sup>42</sup> formulas:

- the first one for the on-shell T matrix  $t(\mathbf{p}' \leftarrow \mathbf{p})$

$$t(\mathbf{p}' \leftarrow \mathbf{p}) = \langle\mathbf{p}'|\widehat{V}|\mathbf{p}\pm\rangle = \langle\mathbf{p}' - |\widehat{V}|\mathbf{p}\rangle, \quad (1.24)$$

- the second one called *Lippmann-Schwinger equation for  $|\mathbf{p}\pm\rangle$* <sup>43</sup>

$$|\mathbf{p}\pm\rangle = |\mathbf{p}\rangle + \widehat{G}_0(E_p \pm i0)\widehat{V}|\mathbf{p}\pm\rangle. \quad (1.25)$$

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<sup>40</sup>The Møller operators are defined at  $\mathcal{H}$ , thus proper definition is

$$|\psi\rangle = \int_{\mathbb{R}} d\mathbf{p} \psi(\mathbf{p})|\mathbf{p}\rangle \implies |\psi\pm\rangle = \widehat{\Omega}_\pm|\psi\rangle = \int_{\mathbb{R}} d\mathbf{p} \psi(\mathbf{p}) \underbrace{\widehat{\Omega}_\pm|\mathbf{p}\rangle}_{=:|\mathbf{p}\pm\rangle}.$$

<sup>41</sup>More detailed procedure can be found in the literature, e.g. Taylor (2006) [6].

<sup>42</sup>The convenience is evident. The scattering system is specified directly by the potential  $\widehat{V}$ , the Lippmann-Schwinger equation for  $|\mathbf{p}\pm\rangle$  provides implicit solution for scattering states  $|\mathbf{p}\pm\rangle$  (the matrix elements of the free Green's operator are known, more at appendix A.1). Using (1.24) we have directly the on-shell T matrix, thus the matrix elements of the scattering operator  $\widehat{S}$ .

<sup>43</sup>In (1.21)

$$\widehat{G}(E_p \pm i0)\widehat{V}|\mathbf{p}\rangle \stackrel{(1.18)}{=} \widehat{G}_0(E_p \pm i0)\widehat{T}(E_p \pm i0)|\mathbf{p}\rangle \stackrel{(1.23)}{=} \widehat{G}_0(E_p \pm i0)\widehat{V}|\mathbf{p}\pm\rangle.$$

## 2. Delta potential and one-channel scattering

Before we solve the two-channel scattering problem, it would be instructive to solve simpler scattering problem (one channel) with two different methods.

First, we calculate eigenvectors for given Hamiltonian  $\hat{H}$  and then we determinate the on-shell matrix elements of T operator. From theory we know direct relationship (1.22) between matrix elements of the on-shell T operator  $\langle k, s' | \hat{T}(E_k + i0) | k, s \rangle$  and the scattering operator  $\langle k, s' | \hat{S} | k, s \rangle$ .

For one-channel one-dimensional scattering problem we assume that the state of particle  $|\psi\rangle \in \mathcal{H}$  is represented (in position representation) by square-integrable wave function  $\psi(x) \in \mathcal{L}^2(\mathbb{R})$ . We assume time-independent Hamiltonian of single non-relativistic particle of mass  $m$  as (expressed in position representation)

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x).$$

By choosing suitable units we can reduce multiplicative constants in equation. This is equivalent setting  $\hbar = 1$  and  $m = 1$ . Our model system will contain Dirac delta function potential (usually shortened as *delta potential*), thus

$$\hat{H} = \underbrace{-\frac{1}{2} \frac{d^2}{dx^2}}_{\hat{H}_0} + \underbrace{\lambda \delta(x)}_{\hat{V}},$$

where  $\lambda$  is parameter of potential strength.

From (1.1) and (1.11) we have eigenvectors  $|k, \pm\rangle$  of the free Hamiltonian  $\hat{H}_0$  with non-negative energy ( $E_k \geq 0$ )

$$\langle x | k, s \rangle = \frac{1}{\sqrt{2\pi}} e^{iskx} \quad \hat{H}_0 |k, s\rangle = \underbrace{\frac{k^2}{2}}_{E_k} |k, s\rangle, \quad (2.1)$$

representing free particle moving right ( $|k, +\rangle$ ) or left ( $|k, -\rangle$ ) along the positive  $x$  coordinate axis, where  $k > 0$  is the magnitude of momentum and  $s = \pm 1$  is the direction of momentum.

### 2.1 Solution of Schrödinger equation – sewing method

In the first place, we will briefly describe main idea of the *sewing method*.

Systems with delta potentials can easily be solved because potential is zero almost everywhere. In these intervals we get solution of time-independent Schrödinger equation for Hamiltonian without potential (free particle). We need to "sew" ("glue") these particular solutions in points  $\{a_j\}$ , where delta potential  $\delta_{a_j}(x) := \delta(x - a_j)$  has origin. This is accomplished by fulfilling two conditions:

1. *Continuity of wave function.* The wave function  $\psi(x)$  is continuous everywhere

$$\lim_{x \rightarrow a_j^-} \psi(x) = \psi(a_j) = \lim_{x \rightarrow a_j^+} \psi(x). \quad (2.2)$$



2. *Step discontinuity in the derivative.* The derivative of the wave function  $\psi'(x)$  has step discontinuity at  $x = a_j$ <sup>1</sup>

$$\lim_{x \rightarrow a_j^+} \psi'(x) - \lim_{x \rightarrow a_j^-} \psi'(x) = 2\lambda\psi(a_j). \quad (2.3)$$

Now more detailed solution is provided for our specific case. In the intervals  $I_- := (-\infty, 0)$  and  $I_+ := (0, +\infty)$  we solve time-independent Schrödinger equation for free particle for function  $\psi(x)$ <sup>2</sup>

$$\left(\widehat{H} - E\right) |\psi\rangle \xrightarrow{\langle x|} -\frac{1}{2} \frac{d^2\psi}{dx^2}(x) - E\psi(x) = 0.$$

Solving homogeneous linear ordinary differential equation (ODE) we attain general solution  $\psi(x)$ <sup>3</sup>

$$-\frac{1}{2}z^2 - E = 0 \implies z_{1,2} = \pm\Lambda = \begin{cases} \pm\sqrt{-2E} & , E < 0 \\ \pm i\sqrt{2E} & , E > 0 \end{cases} \\ \psi(x) = c_{1\pm}e^{z_1x} + c_{2\pm}e^{z_2x}, x \in I_{\pm} \quad (2.4)$$

### 2.1.1 Scattering states

For positive energy ( $E > 0$ ) we define  $k = \sqrt{2E}$ . In the scattering theory we choose these boundary conditions:  $c_{1-} = 1$ ,  $c_{2-} = r$ ,  $c_{1+} = t$ ,  $c_{2+} = 0$ .<sup>4</sup>

Applying boundary conditions (2.2) and (2.3) (where  $a_j = 0$ ) for general solution (2.4) we obtain

$$\left. \begin{aligned} (2.2) \implies 1 + r = \psi(0) &= t \\ (2.3) \implies (ikt - ik0) - (ik1 - ikr) &= 2\lambda\psi(0) \end{aligned} \right\} \implies \begin{cases} r = -\frac{\lambda}{\lambda - ik} \\ t = -\frac{ik}{\lambda - ik} \end{cases},$$

and the complete solution  $\psi(x) \notin \mathcal{L}^2(\mathbb{R})$  is

$$\psi(x) = \begin{cases} e^{+ikx} - \frac{\lambda}{\lambda - ik} e^{-ikx} & , x \leq 0 \\ -\frac{ik}{\lambda - ik} e^{+ikx} & , x \geq 0 \end{cases}, \quad (2.5)$$

for energy  $E = E_k$ .

<sup>1</sup> The second condition arises from the formal integration of time-independent Schrödinger equation in the  $\epsilon$ -neighbourhood ( $a_j - \epsilon, a_j + \epsilon$ ) for  $\epsilon > 0$

$$\int_{a_j - \epsilon}^{a_j + \epsilon} dx \widehat{H}\psi(x) = \underbrace{\int_{a_j - \epsilon}^{a_j + \epsilon} dx \left( -\frac{1}{2}\psi''(x) + \lambda\delta_{a_j}(x)\psi(x) \right)}_{-\frac{1}{2}[\psi'(x)]_{a_j - \epsilon}^{a_j + \epsilon} + \lambda\psi(a_j)} = E \underbrace{\int_{a_j - \epsilon}^{a_j + \epsilon} dx \psi(x)}_{O(\epsilon)}.$$

Using limit  $\epsilon \rightarrow 0^+$  we achieve desired result.

<sup>2</sup>Eigenfunctions  $\psi(x)$  of the Hamiltonian  $\widehat{H}$  does not have to be (and indeed for  $E \geq 0$  they will not be) from space  $\mathcal{L}^2(\mathbb{R})$ .

<sup>3</sup>Solution of ODE is defined on open intervals  $I_{\pm}$  therefore it is not defined in  $x = 0$ .

<sup>4</sup>This choice is motivated by following reasoning. We are looking for solution with only one incoming wave (and outgoing waves with some amplitudes). Incoming waves are  $e^{ikx}$  for  $x < 0$  and  $e^{-ikx}$  for  $x > 0$ . Outgoing waves are  $e^{-ikx}$  for  $x < 0$  and  $e^{ikx}$  for  $x > 0$ . One constant can be chosen without restrain, because any quantum state  $|\psi\rangle$  is represented by ray in Hilbert space  $\{a|\psi\rangle | a \in \mathbb{C} \setminus \{0\}\}$  (or alternatively one multiplicative constant is determined by normalization). We choose  $c_{1-} = 1$  and  $c_{2+} = 0$ . Remaining constants are relabelled  $c_{2-} = r$  (*reflection*),  $c_{1+} = t$  (*transmission*).

### 2.1.2 Bound states

So far we did not treat the case, when energy is negative ( $E < 0$ ). General solution (2.4) has problem with the parts, which in limit ( $x \rightarrow \pm\infty$ ) diverge. This is in contradiction with normalizability. Thus we choose  $c_{2-} = c_{1+} = 0$ .

From sewing conditions (2.2) and (2.3) (where  $a_j = 0$ ) for general solution (2.4) we retrieve

$$\left. \begin{aligned} (2.2) &\implies c_{1-} = \psi(0) = c_{2+} \\ (2.3) &\implies (-\Lambda c_{2+}) - (\Lambda c_{1-}) = 2\lambda\psi(0) \end{aligned} \right\} \implies \left\{ \begin{aligned} c_{1-} = c_{2+} &=: N \\ \Lambda &= -\lambda \end{aligned} \right. .$$

We got for given potential one bound state and only for negative parameter  $\lambda < 0$ . The wave function of the bound state  $\psi(x) \in \mathcal{L}^2(\mathbb{R})$  is<sup>5</sup>

$$\psi(x) = Ne^{\lambda|x|} = \sqrt{-\lambda}e^{\lambda|x|},$$

with energy

$$E_{\text{bound}} = -\frac{\lambda^2}{2}.$$

## 2.2 Solution of Lippmann–Schwinger equation

Alternatively and more quickly, the scattering problem can be solved using Lippmann–Schwinger equation for  $|\mathbf{p}\pm\rangle$ <sup>6</sup> (1.25) in the position representation (using insertion of the spectral decomposition of the unit operator  $\hat{1}$ )

$$\langle x|(k, s)\pm\rangle = \langle x|k, s\rangle + \int_{\mathbb{R}} dx' \langle x|\hat{G}_0(E_k \pm i0)|x'\rangle \langle x'|\hat{V}|(k, s)\pm\rangle. \quad (2.6)$$

From (A.7) we know

$$\langle x|\hat{G}_0(E_k \pm i0)|x'\rangle = \pm \frac{1}{ik} e^{\pm ik|x'-x|},$$

and term  $\langle x'|\hat{V}|(k, s)\pm\rangle$  is straightforward

$$\langle x'|\hat{V}|(k, s)\pm\rangle = \lambda\delta(x')\langle x'|k, s\rangle. \quad (2.7)$$

Applying these changes into the equation (2.6) and using equation (2.1) (notation:  $\psi_{k,s}^{\pm}(x) := \langle x|(k, s)\pm\rangle$ ) we get

$$\psi_{k,s}^{\pm}(x) = \frac{1}{\sqrt{2\pi}} e^{iskx} \pm \frac{\lambda}{ik} e^{\pm ik|x|} \psi_{k,s}^{\pm}(0),$$

where undetermined implicit constant  $\psi_{k,s}^{\pm}(0)$  is determined by setting  $x = 0$

$$\psi_{k,s}^{\pm}(0) = \frac{1}{\sqrt{2\pi}} \pm \frac{\lambda}{ik} \psi_{k,s}^{\pm}(0) \implies \psi_{k,s}^{\pm}(0) = \mp \frac{1}{\sqrt{2\pi}} \frac{ik}{\lambda \mp ik}.$$

The complete solution then is

$$\psi_{k,s}^{\pm}(x) = \frac{1}{\sqrt{2\pi}} \left[ e^{iskx} - \frac{\lambda}{\lambda \mp ik} e^{\pm ik|x|} \right], \quad (2.8)$$

for energy  $E = E_k$ .

Notice that the solution  $\psi_{k,+}^+(x)$  of Lippmann–Schwinger equation (2.5) and the solution  $\psi(x)$  of Schrödinger equation (2.8) differs only by multiplicative constant  $1/\sqrt{2\pi}$  (consequence of different normalization). The other solutions  $\psi_{k,s}^{\pm}(x)$  are equivalent to the solution  $\psi(x)$  of Schrödinger equation with different boundary conditions.

<sup>5</sup>The normalization constant  $N$  was determined using normalization condition  $\langle \psi|\psi\rangle = 1$ .

<sup>6</sup>In three dimensional scattering the Møller operators  $\hat{\Omega}_{\pm}$  related plane wave  $|\mathbf{p}\rangle$  to two improper vectors  $|\mathbf{p}\pm\rangle$ . In one dimensional scattering the corresponding notation for the plane wave is  $|k, s\rangle$  and for two improper vectors  $|(k, s)\pm\rangle$ .

## 2.3 Matrix elements of the scattering operator $S$

As it has been shown in the first chapter (1.22) and (1.24), the matrix elements of the scattering operator  $\widehat{S}$  can be expressed as<sup>7,8</sup>

$$\langle k', s' | \widehat{S} | k, s \rangle = \delta(k' - k) \underbrace{\left[ \delta_{s's} - \frac{2\pi i}{k} \langle k, s' | \widehat{V} | (k, s) + \rangle \right]}_{=: S_{s's}(E_k)},$$

where  $S_{s's}(E_k)$  is called *S matrix*.

Using the same trick (insertion of the unit operator  $\widehat{1}$ ) we obtain for S matrix

$$\begin{aligned} S_{s's}(E_k) &= \delta_{s's} - \frac{2\pi i}{k} \int_{\mathbb{R}} dx \langle k, s' | x \rangle \langle x | \widehat{V} | (k, s) + \rangle \stackrel{(2.7)}{=} \\ &= \delta_{s's} - \frac{2\pi i}{k} \lambda \psi_{k,s'}(0)^* \psi_{k,s}^+(0) = \delta_{s's} - \frac{\lambda}{\lambda - ik} \end{aligned} \quad (2.9)$$

The situation is symmetrical about the origin  $x = 0$ , hence  $S_{s's}(E_k) = S_{-s'-s}(E_k)$  and we need only to evaluate  $S_{s's}$  for one incoming direction ( $s = +1$ ). The resulting probability of transmission  $T := |S_{++}(E_k)|^2$  and probability of reflection  $R := |S_{-+}(E_k)|^2$  as function of  $k$  are

$$T(k) = \frac{k^2}{\lambda^2 + k^2}, \quad R(k) = \frac{\lambda^2}{\lambda^2 + k^2},$$

and expressed in terms of dimensionless energy  $\epsilon := \frac{2E_k}{\lambda^2}$  as

$$T(\epsilon) = \frac{\epsilon}{1 + \epsilon}, \quad R(\epsilon) = \frac{1}{1 + \epsilon}.$$

Easy check gives us total probability equal to  $T(E_k) + R(E_k) = 1$ . We can see, that for any  $\lambda$  the energy can be rescaled into the units  $\frac{\lambda^2}{2}$  and in terms of  $T(E_k)$  and  $R(E_k)$  there is only one delta potential one-channel scattering model without any parameters.

<sup>7</sup>The term  $\delta(E_{k'} - E_k)$  from (1.22) can be expressed in terms of  $k$  and  $k'$ : The free Hamiltonian  $\widehat{H}_0$  has orthogonal bases  $|E, \alpha\rangle$  and  $|k, \alpha\rangle$  normalized to Dirac delta function as follows

$$\begin{aligned} |E, \alpha\rangle : \widehat{1} &= \sum_{\alpha} \int_E dE |E, \alpha\rangle \langle E, \alpha| & \delta(E' - E) &= \sum_{\alpha} \langle E', \alpha | E, \alpha \rangle, \\ |k, \alpha\rangle : \widehat{1} &= \sum_{\alpha} \int_k dk |k, \alpha\rangle \langle k, \alpha| & \delta(k' - k) &= \sum_{\alpha} \langle k', \alpha | k, \alpha \rangle. \end{aligned}$$

The improper vectors  $|E_k, \alpha\rangle$  and  $|k, \alpha\rangle$  differ only by some normalization constant  $N(k, \alpha)$

$$|E_k, \alpha\rangle = N(k, \alpha) |k, \alpha\rangle.$$

Using substitution  $E = \frac{k^2}{2}$  we can transform one spectral decomposition of unit operator to other one

$$dE |E, \alpha\rangle \langle E, \alpha| = dk \underbrace{\left[ \frac{dE}{dk} \right]}_k |N(k, \alpha)|^2 |k, \alpha\rangle \langle k, \alpha| = dk |k, \alpha\rangle \langle k, \alpha|.$$

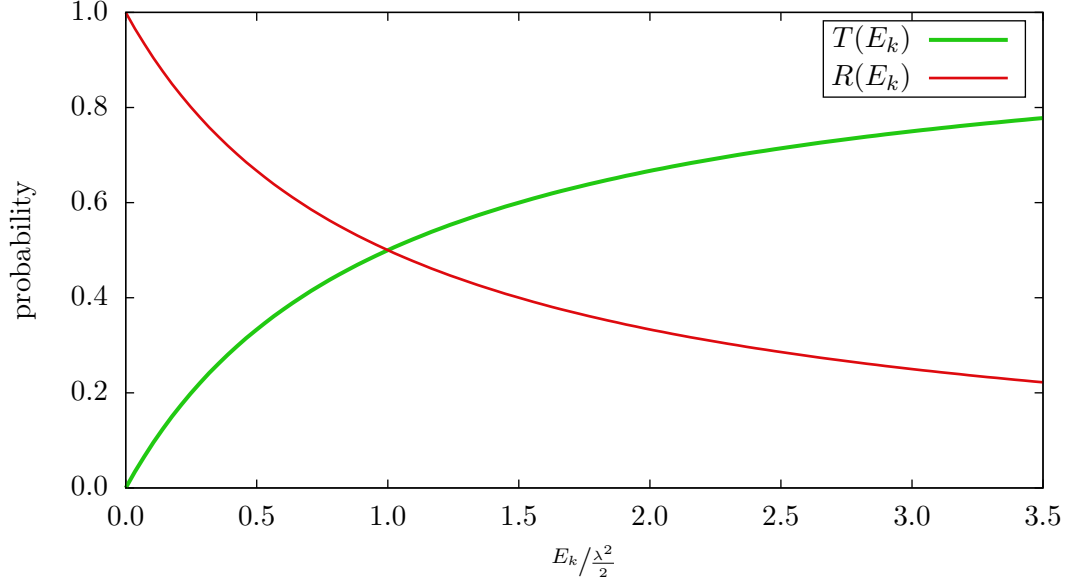
We get formula for normalization constant  $N(k, \alpha)$  (determined up to phase, we chose real non-negative constant)

$$N(k, \alpha) = \frac{1}{\sqrt{k}}.$$

and for the term  $\delta(E_{k'} - E_k)$  we get

$$\delta(E_{k'} - E_k) = \sum_{\alpha} \langle E_{k'}, \alpha | E_k, \alpha \rangle = \frac{1}{\sqrt{k'k}} \sum_{\alpha} \langle k', \alpha | k, \alpha \rangle = \frac{1}{\sqrt{k'k}} \delta(k' - k) = \frac{1}{k} \delta(k' - k).$$

<sup>8</sup>The on-shell matrix elements of T operator can be evaluated as  $\langle k', s' | \widehat{V} | (k, s) + \rangle$  or  $\langle (k', s') - | \widehat{V} | k, s \rangle$ . We chose the first option.



**Figure 2.1:** The probability of transmission  $T(E_k)$  and the probability of reflection  $R(E_k)$  as a function of energy of particle  $E_k$ .

We can notice that transmission and reflection is not influenced by the sign of the parameter  $\lambda$  and the scattering properties are same for delta potential well ( $\lambda < 0$ ) and delta potential barrier  $\lambda > 0$  of the same  $|\lambda|$ .

### 2.3.1 Eigenphases

In order to find the eigenphases  $\delta_n$ , we need to find eigenvalues of S matrix. We notice that the parity operator  $\hat{P}$  commutes with the full Hamiltonian  $[\hat{H}, \hat{P}] = 0$ , therefore situation is same for the unitary operator  $[\hat{U}(t), \hat{P}] = 0$ , the Møller operators  $[\hat{\Omega}_\pm, \hat{P}] = 0$  and also for the scattering operator  $[\hat{S}, \hat{P}] = 0$ . Therefore we can choose common set of eigenfunctions. The parity operator  $\hat{P}$  has 2 eigenvalues  $\lambda = \pm 1$  and 2 types of eigenfunctions: *even* ( $\lambda = +1$ ) and *odd* ( $\lambda = -1$ ).<sup>9</sup> The symmetry adapted linear combinations of the functions  $\langle x|k, s \rangle$  are

$$\begin{aligned}\langle x|\psi_1\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ikx} + \frac{1}{\sqrt{2\pi}} e^{-ikx} \right) = \frac{1}{\sqrt{\pi}} \cos(kx), \\ \langle x|\psi_2\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ikx} - \frac{1}{\sqrt{2\pi}} e^{-ikx} \right) = \frac{i}{\sqrt{\pi}} \sin(kx).\end{aligned}$$

The change-of-basis matrix  $Q$  and the inverse matrix  $Q^{-1}$  are<sup>10</sup>

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad Q^{-1} = Q^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

The new S matrix  $S'(k)$  in the new basis is

$$S' = QSQ^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{\lambda - ik} \begin{pmatrix} -ik & -\lambda \\ -\lambda & -ik \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} -\frac{\lambda+ik}{\lambda-ik} & 0 \\ 0 & 1 \end{pmatrix}.$$

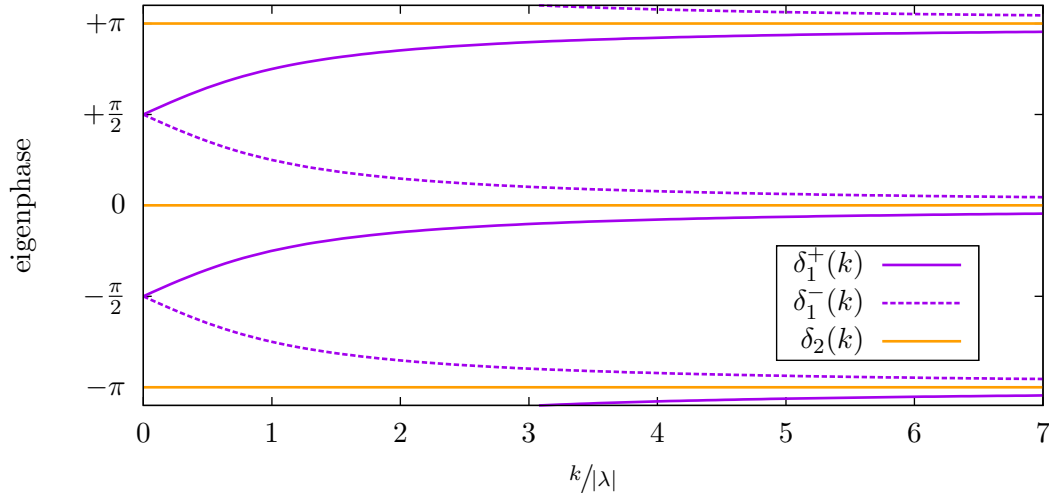
<sup>9</sup>This can be shown simply from the property  $\hat{P}^2 = \hat{1}$ .

<sup>10</sup>For unitary matrix the inverse is  $Q^{-1} = Q^+$ .

This gives us two eigenphases<sup>11</sup>

$$\delta_1(k) \equiv \frac{1}{2} \arg \left( -\frac{\lambda + ik}{\lambda - ik} \right) \equiv \arctan \left( \frac{k}{\lambda} \right) + \frac{\pi}{2} \pmod{\pi}, \quad \delta_2(k) \equiv 0 \pmod{\pi}. \quad (2.10)$$

The momentum dependence of the eigenphases  $\delta_1(k)$  and  $\delta_2(k)$  have been plotted in Figure 2.2 with respect to modulo  $\pi$  ambiguity.



**Figure 2.2:** The eigenphases  $\delta_1^+(k)$  (for  $\lambda > 0$ ),  $\delta_1^-(k)$  (for  $\lambda < 0$ ) and  $\delta_2(k)$  as a function of magnitude of momentum of particle  $k$ .

In the second case, the delta potential is "invisible" for the sine wave  $\langle x|\psi_2\rangle$ . The boundary conditions (2.2) and (2.3) are full-filled for any  $\lambda$ , thus presence ( $\lambda \neq 0$ ) or absence ( $\lambda = 0$ ) of the delta potential does not change the solution.<sup>12</sup>

In the scattering theory of spherical potentials, the problem can be transformed into one-dimensional radial Schrödinger equation and in the low-energy limit there is defined quantity called *scattering length*  $a$ .<sup>13</sup> The meaning: At low energies the differential cross section is  $\frac{d\sigma}{d\Omega} = a^2$ . The scattering length  $a$  appears in the low-energy limit of eigenphase  $\delta(k)$  as (from Taylor (2006), p. 194 [6])

$$\delta(k) \xrightarrow{k \rightarrow 0} \left( n_0 + \frac{1}{2} \right) \pi - ak. \quad (2.11)$$

For our model we get

$$\delta_1(k) \xrightarrow{k \rightarrow 0} \frac{\pi}{2} + \frac{k}{\lambda} \implies a_1 = -\frac{1}{\lambda}. \quad (2.12)$$

<sup>11</sup>To be complete for  $\lambda = 0$ :  $\delta_1(k) \equiv 0 \pmod{\pi}$ .

<sup>12</sup>In general, we know from the boundary conditions (2.2) and (2.3) that is true for any wave function with zero magnitude in the origin and continuous first derivative in the origin.

<sup>13</sup>This quantity can be defined for any orbital quantum number  $l$ , but only for  $l = 0$  is it has the dimension of length.

# 3. Delta function potential and two-channel scattering

In the second chapter we have shown approach how to solve one-channel scattering problem. As the title of chapter suggests, we will be dealing with two-channel scattering problem with delta function potential using same method.

For two-channel one-dimensional scattering problem we assume that the state of particle  $|\psi\rangle \in \mathcal{H} \oplus \mathcal{H} \equiv \mathcal{H} \otimes \mathbb{C}^2$  is represented (in position representation) by ordered pair  $\langle x|\psi\rangle = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}$  of two square-integrable wave functions  $\psi_{1,2}(x) \in \mathcal{L}^2(\mathbb{R})$ .

We made the same assumptions about the Hamiltonian (time-independent non-relativistic Hamiltonian of single spinless particle in one dimension with local delta potential) and about units ( $\hbar = 1$  and  $m = 1$ ), thus

$$\hat{H} = \underbrace{-\frac{1}{2} \frac{d^2}{dx^2} + \begin{pmatrix} 0 & 0 \\ 0 & W \end{pmatrix}}_{\hat{H}_0} + \underbrace{\begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \delta(x)}_{\hat{V}}, \quad (3.1)$$

where  $W$  is the energy difference of channels and  $a, b, c$  are parameters of the potential. Since the Hamiltonian is a self-adjoint operator, elements of main diagonal  $a, b$  are real  $a, b \in \mathbb{R}$  and off-diagonal elements are mutually the complex conjugate.

The free Hamiltonian  $\hat{H}_0$  in every channel has same form as one-dimensional free Hamiltonian (except for additional constant  $W$ ). Therefore using (1.1) and (1.11) the eigenvectors of the free Hamiltonian  $\hat{H}_0$  are

$$\langle x|k_n, s, n\rangle = \frac{1}{\sqrt{2\pi}} e^{isk_n x} \underbrace{\begin{pmatrix} \delta_{1n} \\ \delta_{2n} \end{pmatrix}}_{=: \hat{e}_n} \quad \hat{H}_0 |k_n, s, n\rangle = \underbrace{\left( \frac{k_n^2}{2} + W \delta_{2n} \right)}_E |k_n, s, n\rangle, \quad (3.2)$$

for particle in  $n$ -th channel with the magnitude of momentum  $k_n > 0$  and the direction of momentum  $s = \pm 1$ .

While working on this thesis, we have found the article from Exner (1991) [5] about equivalent two-channel scattering model. The model is solved on positive  $x$ -axis  $\mathbb{R}_+$  and the delta-potential interaction is realised by mathematically more rigorous self-adjoint extension. The correspondence between our notation and notation of the article is following

$$W \leftrightarrow E, \quad a/\sqrt{2} \leftrightarrow a, \quad b/\sqrt{2} \leftrightarrow b, \quad c/\sqrt{2} \leftrightarrow c, \quad \sqrt{2}x \leftrightarrow r.$$

## 3.1 Solution of Lippmann–Schwinger equation

We will use already familiar procedure starting with Lippmann–Schwinger equation for  $|\mathbf{p}\pm\rangle$

$$\langle x|(k_n, s, n)\pm\rangle = \langle x|k_n, s, n\rangle + \int_{\mathbb{R}} dx' \langle x|\hat{G}_0(E \pm i0)|x'\rangle \langle x'|\hat{V}|(k_n, s, n)\pm\rangle. \quad (3.3)$$

The term  $\langle x|\hat{G}_0(E \pm i0)|x'\rangle$  for two-channel scattering is analogous to (A.7) and (A.9)

$$\langle x|\hat{G}_0(E \pm i0)|x'\rangle = \begin{pmatrix} \frac{1}{\pm ik_1} e^{\pm ik_1|x-x'|} & 0 \\ 0 & \frac{1}{K_2} e^{K_2|x-x'|} \end{pmatrix}, \quad (3.4)$$

where

$$K_2 = K_2(E \pm i0) := \begin{cases} \pm ik_2 & , E \geq W \\ -\kappa_2 & , W > E \geq 0 \end{cases} ,$$

and  $k_1 = \sqrt{2E}$ ,  $k_2 = \sqrt{2(E - W)}$  and  $\kappa_2 = \sqrt{2(W - E)}$ .

As before, the term  $\langle x' | \widehat{V} | (k_n, s, n) \pm \rangle$  is simple to express

$$\langle x' | \widehat{V} | (k_n, s, n) \pm \rangle = \delta(x') \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \langle x' | (k_n, s, n) \pm \rangle. \quad (3.5)$$

By inserting the terms (3.4), (3.5) and (3.3) and simpler notation<sup>1</sup> we obtain

$$\begin{pmatrix} \psi_{1(k_n, s, n)}^\pm(x) \\ \psi_{2(k_n, s, n)}^\pm(x) \end{pmatrix} = \frac{\hat{e}_n}{\sqrt{2\pi}} e^{isk_n x} + \begin{pmatrix} \frac{1}{\pm ik_1} e^{\pm ik_1 |x|} & 0 \\ 0 & \frac{1}{K_2} e^{K_2 |x|} \end{pmatrix} \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \begin{pmatrix} \psi_{1(k_n, s, n)}^\pm(0) \\ \psi_{2(k_n, s, n)}^\pm(0) \end{pmatrix}. \quad (3.6)$$

Again, the undetermined implicit constants  $\psi_{1(k_n, s, n)}^\pm(0)$  and  $\psi_{2(k_n, s, n)}^\pm(0)$  are determined from equation for  $x = 0$

$$\xrightarrow[x=0]{(3.6)} \begin{pmatrix} \psi_{1(k_n, s, n)}^\pm(0) \\ \psi_{2(k_n, s, n)}^\pm(0) \end{pmatrix} = \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{\pm ik_1} & 0 \\ 0 & \frac{1}{K_2} \end{pmatrix} \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \right]^{-1} \frac{\hat{e}_n}{\sqrt{2\pi}}.$$

For the invertible matrix  $2 \times 2$  the inverted matrix is

$$M^{-1} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \frac{1}{\det M} \begin{pmatrix} D & -B \\ -C & A \end{pmatrix}, \quad \det M = AD - BC, \quad (3.7)$$

assuming non-zero determinant ( $\det M \neq 0$ ). Using formula (3.7) we get

$$\begin{pmatrix} \psi_{1(k_n, s, n)}^\pm(0) \\ \psi_{2(k_n, s, n)}^\pm(0) \end{pmatrix} = -\frac{1}{\sqrt{2\pi} \Delta_\pm} \begin{pmatrix} \pm ik_1(b - K_2) & -cK_2 \\ \mp ic^*k_1 & K_2(a \mp ik_1) \end{pmatrix} \hat{e}_n, \quad (3.8)$$

where  $\Delta_\pm := (a \mp ik_1)(b - K_2) - |c|^2$ .

As we have seen in the second chapter (2.9), for the matrix elements of the scattering operator  $S$  we need only the value of wave function  $\psi_{1,2(k_n, s, n)}^\pm(x)$  at  $x = 0$ .

---

<sup>1</sup>  $\begin{pmatrix} \psi_{1(k_n, s, n)}^\pm(x) \\ \psi_{2(k_n, s, n)}^\pm(x) \end{pmatrix} := \langle x | (k_n, s, n) \pm \rangle$

### 3.2 Matrix elements of the scattering operator $S$

Analogously to the one-channel we can define two-channel S matrix  $S_{(s'n')(sn)}(E)$  as<sup>2,3</sup>

$$S_{(s'n')(sn)}(E) := \delta_{s's}\delta_{n'n} - \frac{2\pi i}{\sqrt{k_n k_{n'}}} \langle k_{n'}, s', n' | \widehat{V} | (k_n, s, n) \rangle.$$

After the insertion of the identity operator  $\widehat{I}$  we get

$$\begin{aligned} S_{(s'n')(sn)}(E) &= \delta_{s's}\delta_{n'n} - \frac{2\pi i}{\sqrt{k_n k_{n'}}} \int_{\mathbb{R}} dx \langle k_{n'}, s', n' | x \rangle \langle x | \widehat{V} | (k_n, s, n) \rangle \stackrel{(3.5)}{=} \\ &= \delta_{s's}\delta_{n'n} - \frac{2\pi i}{\sqrt{k_n k_{n'}}} \begin{pmatrix} \psi_1(k_{n'}, s', n')(0) \\ \psi_2(k_{n'}, s', n')(0) \end{pmatrix}^+ \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \begin{pmatrix} \psi_1^+(k_n, s, n)(0) \\ \psi_2^+(k_n, s, n)(0) \end{pmatrix} \end{aligned}$$

Using (3.2) and (3.8) we obtain

$$S_{(s'n')(sn)}(E) = \delta_{s's}\delta_{n'n} + \frac{i}{\Delta_+ \sqrt{k_n k_{n'}}} M_{n'n}, \quad (3.9)$$

where  $M$  is matrix  $2 \times 2$  defined as

$$M := \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \begin{pmatrix} ik_1(b - K_2) & -cK_2 \\ -ic^*k_1 & K_2(a - ik_1) \end{pmatrix} = \begin{pmatrix} ik_1(D - aK_2) & ck_1k_2 \\ c^*k_1k_2 & k_2(iD + bk_1) \end{pmatrix},$$

where  $D := ab - |c|^2$ .<sup>4</sup>

For  $c = 0$  we obtain

$$S_{(s'n')(sn)}(E) = \delta_{s's}\delta_{n'n} - \begin{pmatrix} \frac{a}{a-ik_1} & 0 \\ 0 & \frac{b}{b-ik_2} \end{pmatrix}, \quad (3.10)$$

<sup>2</sup>As in one-channel case the free Hamiltonian  $\widehat{H}_0$  has orthogonal bases  $|E_n, \alpha, n\rangle$  and  $|k, \alpha, n\rangle$

$$\begin{aligned} |E, \alpha, n\rangle : \widehat{1} &= \sum_{\alpha} \int_0^{+\infty} dE |E, \alpha, 1\rangle \langle E, \alpha, 1| + \sum_{\alpha} \int_W^{+\infty} dE |E, \alpha, 2\rangle \langle E, \alpha, 2|, \\ |k_n, \alpha, n\rangle : \widehat{1} &= \sum_{\alpha} \int_0^{+\infty} dk_1 |k_1, \alpha, 1\rangle \langle k_1, \alpha, 1| + \sum_{\alpha} \int_0^{+\infty} dk_2 |k_2, \alpha, 2\rangle \langle k_2, \alpha, 2|. \end{aligned}$$

The improper vectors  $|E, \alpha, n\rangle$  and  $|k_n, \alpha, n\rangle$  differ only by normalization constant  $N(k_n, \alpha, n)$

$$|E, \alpha, n\rangle = N(k_n, \alpha, n) |k_n, \alpha, n\rangle.$$

Using substitutions  $E = \frac{k_1^2}{2}$  and  $E = \frac{k_2^2}{2} + W$  we can transform one spectral decomposition of unit operator to other one

$$dE |E, \alpha, n\rangle \langle E, \alpha, n| = dk_n \underbrace{\left| \frac{dE}{dk_n} \right|}_{k_n} |N(k_n, \alpha, n)|^2 |k_n, \alpha, n\rangle \langle k_n, \alpha, n| = dk_n |k_n, \alpha, n\rangle \langle k_n, \alpha, n|.$$

We get formula for normalization constant  $N(k_n, \alpha, n)$  (determined up to phase, we chose real non-negative constant)

$$N(k_n, \alpha, n) = \frac{1}{\sqrt{k_n}}.$$

and for the term  $\delta(E' - E)$  we get

$$\delta(E' - E) = \sum_{\alpha, n} \langle E', \alpha, n | E, \alpha, n \rangle = \frac{1}{\sqrt{k_n' k_n}} \sum_{\alpha, n} \langle k_n', \alpha, n | k_n, \alpha, n \rangle.$$

<sup>3</sup>As before, we can use  $\langle k_{n'}, s', n' | \widehat{V} | (k_n, s, n) \rangle$  or  $\langle (k_{n'}, s', n') - | \widehat{V} | k_n, s, n \rangle$ . Both options lead to the same result. We chose the first one.

<sup>4</sup>The term  $\delta(E' - E)$  in (1.22) allows for elements with energy  $E \geq W$  to specify  $K_2$  as  $ik_2$ .



which agrees with the one-channel scattering result (2.9).

As before, the task is symmetrical about  $x = 0$  ( $S_{(s'n')(sn)}(E) = S_{(-s'n')(-sn)}(E)$ ), thus it is necessary to evaluate only for one direction, for instance  $s = +1$ . We define the probability of transmission [reflection] from the  $n$ -th channel to the  $n'$ -channel  $T_{n'n}(E)$  [ $R_{n'n}(E)$ ] as<sup>5</sup>

$$T_{n'n}(E) := |S_{(sn')(sn)}(E)|^2, \quad R_{n'n}(E) := |S_{(-sn')(sn)}(E)|^2.$$

Our interest is focused on situation with particle incoming in the first channel ( $n = 1$ ).

We can notice that  $T_{21}(E)$  and  $R_{21}(E)$  are same. This is expectable, because coupling between two channels is provided by the delta potential, which effectively mediates only the value of wave function in the origin  $x = 0$ , but nothing else (not even the direction of the incoming particle).<sup>6</sup> Thus the solution in the second channel must be symmetrical.

As verification of the unitarity of S matrix we can check probability conservation.

$$T_{11}(E) + R_{11}(E) + T_{21}(E) + R_{21}(E) = 1.$$

For  $W > E > 0$  we get

$$\underbrace{\left|1 - \frac{D + a\kappa_2}{\Delta_+}\right|^2}_{T_{11}} + \underbrace{\left|\frac{D + a\kappa_2}{\Delta_+}\right|^2}_{R_{11}} + \underbrace{0}_{T_{21}+R_{21}} = \frac{|-ik_1(b + \kappa_2)|^2 + |D + a\kappa_2|^2}{|D + a\kappa_2 - ik_1(b + \kappa_2)|^2} = 1,$$

where in the last step we just need to notice that there is the sum of squares of imaginary and real part of some complex number in the numerator and there is the square of the absolute value of the same complex number in the denominator (the Pythagorean theorem).

For  $E > W$  we get

$$\begin{aligned} & \underbrace{\left|1 - \frac{D - iak_2}{\Delta_+}\right|^2}_{T_{11}} + \underbrace{\left|\frac{D - iak_2}{\Delta_+}\right|^2}_{R_{11}} + 2 \underbrace{\left|\frac{c^* \sqrt{k_1 k_2}}{\Delta_+}\right|^2}_{T_{21}+R_{21}} = \\ & = \frac{\left[(k_1 k_2)^2 + (bk_1)^2\right] + \left[D^2 + (ak_2)^2\right] + 2|c|^2 k_1 k_2}{\left[D^2 + (-2Dk_1 k_2) + (k_1 k_2)^2\right] + \left[(bk_1)^2 + 2abk_1 k_2 + (ak_2)^2\right]} = 1. \end{aligned}$$

This model has 5 real parameters:  $W$ ,  $a$ ,  $b$  and  $c = |c|e^{i\phi}$ . But it is possible to express energy in the units  $W$  and rescale variable  $x \rightarrow \frac{x}{\sqrt{W}}$ , which is equivalent setting  $W = 1$ . Also the phase  $\phi$  of the constant  $c$  does not occur in terms of  $T_{n'n}(E)$  and  $R_{n'n}(E)$ .<sup>7</sup> The delta potential two-channel scattering model has 3 free parameters:  $a$ ,  $b$  and  $|c|$ .

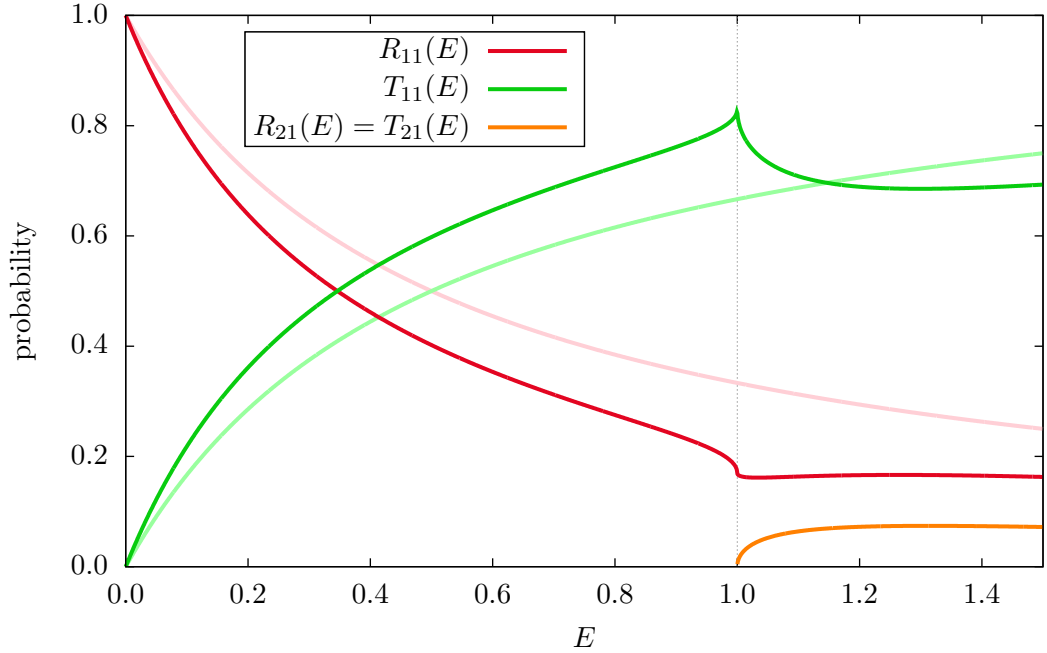
To get better insight we plotted the energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  for a few values. Colour coding of curves is explained in Figure 3.1.  $T(E)$  and  $R(E)$  represent the scattering for uncoupled case (see (3.10)), the background scattering<sup>8</sup>

<sup>5</sup>It is important to note, that this holds only for open channels. For instance, for  $W > E > 0$  matrix elements  $S_{(s'2)(+1)}$  are technically non-zero, but from the energy point of view the second channel is closed.

<sup>6</sup>This can be illustrated in the 2D plane. The first and the second channel can be identified with  $x$  axis and  $y$  axis, respectively. The particle incoming from the positive  $x$  axis has same probability to go to the positive and to the negative  $y$  axis.

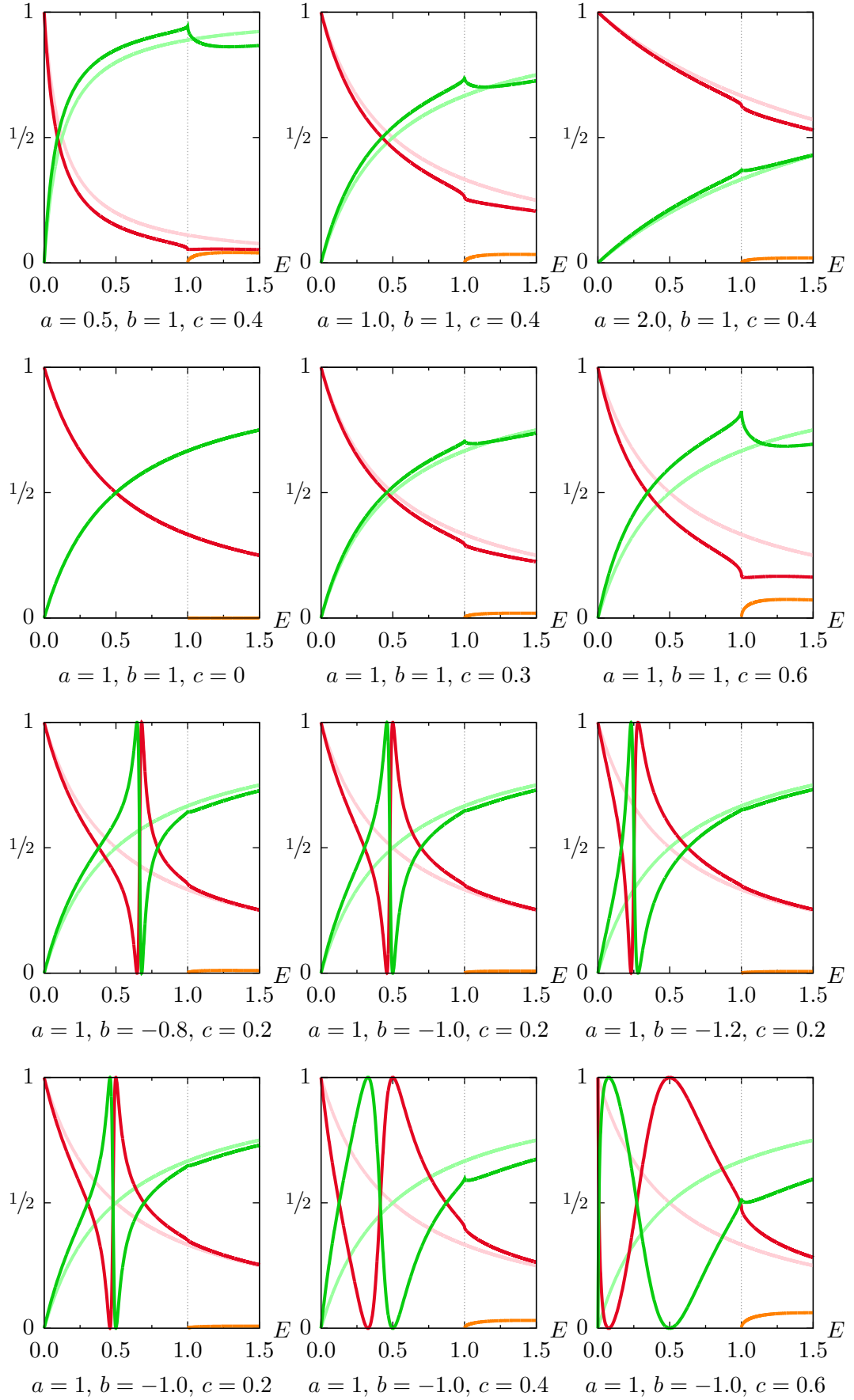
<sup>7</sup>The phase  $\phi$  only shifts the phase of the outgoing waves, thus it does not affect the probability. Also the phase of  $c$  can be eliminated by the suitable choice of phases of base vectors  $\hat{e}_1$  and  $\hat{e}_2$ .

<sup>8</sup>This background scattering is different from the background scattering in the projection-operation formalism.



**Figure 3.1:** The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  for parameters:  $a = 1$ ,  $b = 1$ ,  $|c| = 0.6$  with marked threshold energy  $W = 1$  (dashed line) and the probabilities  $T(E)$  and  $R(E)$  of one-channel scattering for  $\lambda = a$  for comparison (equivalent to no coupling  $|c| = 0$ ).

**Rough insight into the effects of parameters.** In every row of Figure 3.2 we change the value of one parameter, while the others are fixed. In the first row, we can see that the parameter  $a$  determines increasing and decreasing rate of  $T(E)$  and  $R(E)$  respectively, relatively to the threshold energy  $W = 1$ . In the second row, we observe that the parameter  $|c|$  determines strength of coupling (for  $|c| = 0$  there is no interaction) and affects the magnitude of cusps. The common behaviour in this two-channel model is the presence of cusps around threshold  $E = W = 1$  (typical threshold behaviour). This phenomenon can be more or less seen in every figure for any settings of parameters (only for the trivial uncoupled case  $|c| = 0$  this effect is not present). In the third and fourth row, we see that parameters  $b$  and  $|c|$  determine the presence (both), position (mainly  $b$ ; the 3rd row) and width (mainly  $|c|$ ; the 4th row) of resonances. The resonances will be studied in more detail in the following section as analytical properties of S matrix.



**Figure 3.2:** The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  for various settings of parameters with marked threshold energy  $W = 1$  (dashed line) and the no-coupling probabilities  $T(E)$  and  $R(E)$ .

### 3.2.1 Eigenphases

As already seen in the previous chapter for the one-channel model, the commutativity of the parity operator  $\hat{P}$  and the full Hamiltonian  $\hat{H}$  ( $[\hat{H}, \hat{P}] = 0$ ) helps to find the eigenphases  $\delta_n$  (eigenvalues of S matrix). In the same manner this commutativity implies commutative relation  $[\hat{S}, \hat{P}] = 0$  and we can choose common set of eigenfunctions. The symmetry adapted linear combinations of the functions  $\langle x|k_n, s, n\rangle$  are

$$\begin{aligned}\langle x|\psi_1\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ik_1x} + \frac{1}{\sqrt{2\pi}} e^{-ik_1x} \right) \hat{e}_1 = \frac{1}{\sqrt{\pi}} \cos(k_1x) \hat{e}_1, \\ \langle x|\psi_2\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ik_1x} - \frac{1}{\sqrt{2\pi}} e^{-ik_1x} \right) \hat{e}_1 = \frac{i}{\sqrt{\pi}} \sin(k_1x) \hat{e}_1, \\ \langle x|\psi_3\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ik_2x} + \frac{1}{\sqrt{2\pi}} e^{-ik_2x} \right) \hat{e}_2 = \frac{1}{\sqrt{\pi}} \cos(k_2x) \hat{e}_2, \\ \langle x|\psi_4\rangle &:= \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{2\pi}} e^{ik_2x} - \frac{1}{\sqrt{2\pi}} e^{-ik_2x} \right) \hat{e}_2 = \frac{i}{\sqrt{\pi}} \sin(k_2x) \hat{e}_2.\end{aligned}$$

We must not forget that the dimensionality of the S matrix depends on the energy: for  $W > E > 0$  it is  $2 \times 2$ , for  $E > W$  it is  $4 \times 4$ . When the second channel is closed, we will use for base only first two symmetry adapted functions  $\langle x|\psi_i\rangle$ .

The change-of-basis matrix  $Q$  and the inverse matrix  $Q^{-1}$  are

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \quad Q^{-1} = Q^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}.$$

The new S matrix  $S'$  in the new basis is

$$S' = QSQ^{-1} = \begin{cases} \begin{pmatrix} \left( \frac{-D - a\kappa_2 - ik_1b - ik_1\kappa_2}{+D + a\kappa_2 - ik_1b - ik_1\kappa_2} \right) & 0 \\ 0 & 1 \end{pmatrix} & , W > E > 0 \\ \begin{pmatrix} \left( \frac{-D - k_1k_2 - ik_1b + ik_2a}{+D - k_1k_2 - ik_1b - ik_2a} \right) & 0 & \frac{2ic\sqrt{k_1k_2}}{+D - k_1k_2 - ik_1b - ik_2a} & 0 \\ 0 & 1 & 0 & 0 \\ \frac{2ic^*\sqrt{k_1k_2}}{+D - k_1k_2 - ik_1b - ik_2a} & 0 & \frac{-D - k_1k_2 + ik_1b - ik_2a}{+D - k_1k_2 - ik_1b - ik_2a} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & , E > W \end{cases}.$$

For the case  $W > E > 0$  the corresponding eigenphases are

$$\delta_1(k_1) \equiv \frac{1}{2} \arg \left( \frac{-D - a\kappa_2 - ik_1b - ik_1\kappa_2}{+D + a\kappa_2 - ik_1b - ik_1\kappa_2} \right) \pmod{\pi}, \quad \delta_2(k_1) \equiv 0 \pmod{\pi}.$$

As before, for the sine waves  $\langle x|\psi_2\rangle$  and  $\langle x|\psi_4\rangle$  the potential is "invisible" and the corresponding eigenphases  $\delta_2(k_1)$  and  $\delta_4(k_1)$  are zero for any energy  $E$

$$\delta_2(k_1) \equiv 0 \pmod{\pi}, \quad \delta_4(k_1) \equiv 0 \pmod{\pi}.$$

For the case  $E > W$  the task of finding the eigenvalues is not complete and using the standard technique (*characteristic polynomial*) leads to quadratic equation. The corresponding eigenphases are<sup>9</sup>

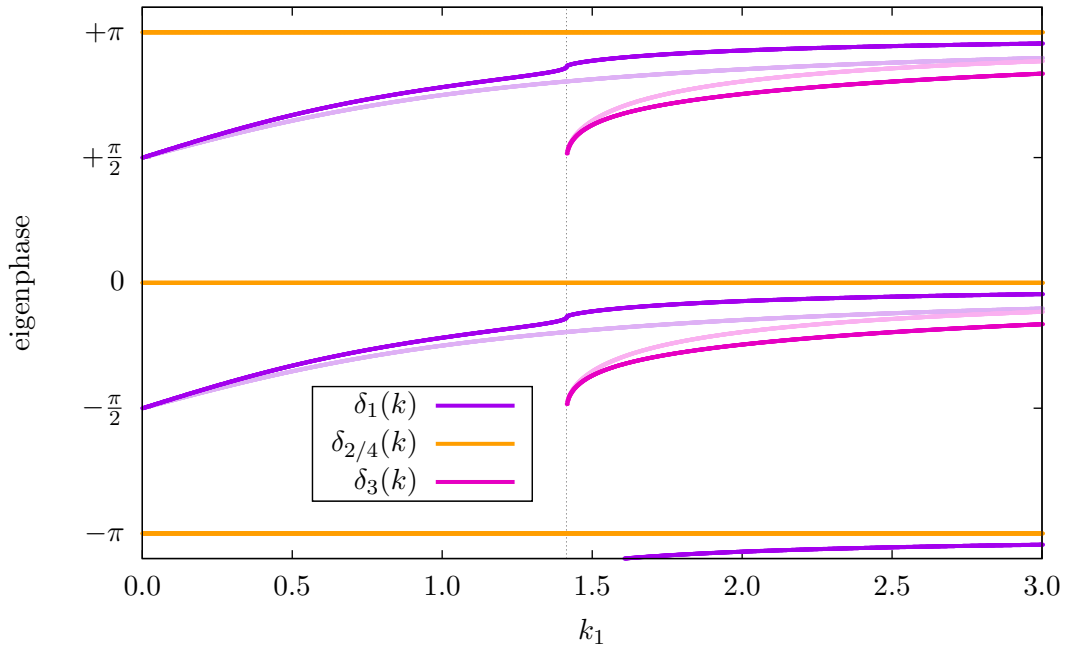
$$\delta_{1/3}(k_1) \equiv \frac{1}{2} \arg \left( \frac{-D - k_1k_2 \mp \text{sgn}(b)i\sqrt{(k_1b - k_2a)^2 + 4|c|^2k_1k_2}}{D - k_1k_2 - ik_1b - ik_2a} \right) \pmod{\pi}.$$

<sup>9</sup>The term  $\text{sgn}(b)$  is present, so the eigenphase  $\delta_1(k_1)$  is continuous at threshold  $k_1 = \sqrt{2W}$ .

For no coupling  $c = 0$  we get eigenphases corresponding to one-dimensional case (2.10)

$$\begin{aligned}\delta_1^0 &\equiv \frac{1}{2} \arg \left( \frac{-a - ik_1}{a - ik_1} \right) \pmod{\pi}, & \delta_2^0 &\equiv 0 \pmod{\pi}, \\ \delta_3^0 &\equiv \frac{1}{2} \arg \left( \frac{-b - ik_2}{b - ik_2} \right) \pmod{\pi}, & \delta_4^0 &\equiv 0 \pmod{\pi}.\end{aligned}$$

To understand better the eigenphases we plotted the  $k_1$ -momentum dependence of the eigenphases  $\delta_i(k_1)$  for a few values. In Figure 3.3 we can see common key for all plotted dependences.



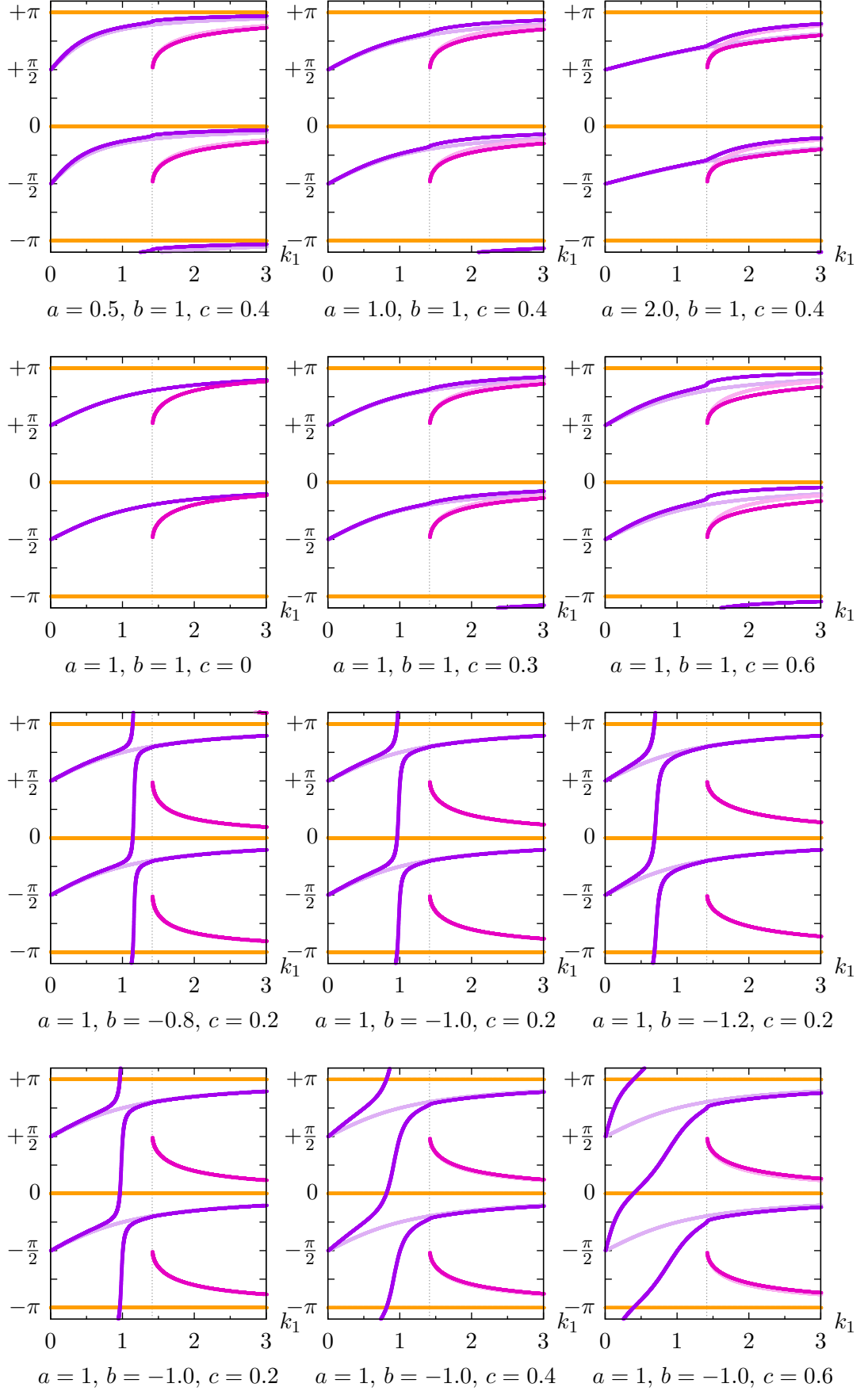
**Figure 3.3:** The eigenphases  $\delta_i(k_1)$  for parameters:  $a = 1$ ,  $b = 1$ ,  $|c| = 0.6$  with marked threshold momentum  $k_1 = \sqrt{2W}$  (dashed line) and no-coupling eigenphases  $\delta_i^0(k_1)$  for comparison (pale lines).

In Figure 3.4 we get same rough insight based on the eigenphases into the effects of parameters as before in Figure 3.2 based on the probabilities. The resonances can be seen as the rapid changes in eigenphase and they are directly linked to quick  $+\pi$  change, which graphically means shift to the next  $\pi$ -wide strip (modulo  $\pi$  ambiguity of eigenphase; the third and the fourth row of Figure 3.4).

As before in the one-channel scattering model, we can define in the low-energy limit *scattering length*  $a$  and using the relation (2.11) we get

$$\delta_1(k_1) \xrightarrow{k_1 \rightarrow 0} \frac{\pi}{2} + \frac{b + \sqrt{2W}}{D + a\sqrt{2W}} k_1 \implies a_1 = -\frac{b + \sqrt{2W}}{a(b + \sqrt{2W}) - |c|^2}.$$

For no coupling  $c = 0$  we can see agreement with the one-channel relation (2.12).



**Figure 3.4:** The eigenphases  $\delta_i(k_1)$  for various settings of parameters with marked threshold momentum  $k_1 = \sqrt{2W}$  (dashed line) and the no-coupling eigenphases  $\delta_i^0(k_1)$  (pale lines).

### 3.3 Poles of the S matrix

From theory (for instance Taylor (2006), chapter 13 "Resonances" [6]) we know, that if we extend the matrix elements of the scattering operator  $\widehat{S}$  from function of real variable  $k_1 \geq 0$  to analytic function of the complex variable  $k_1$ , then the poles of the S matrix correspond to some important states of the system.

Analytic functions have an important property: If two analytic functions coincide on some line segment, then they coincide everywhere.<sup>10</sup> This allows us *unique analytic continuation* of any analytic (differentiable) function defined on some line segment of real axis into complex plane. From (3.9) we know matrix elements  $S_{(s'n')(sn)}(k_1)$  as functions of non-negative real  $k_1$ . They are differentiable on intervals  $(0, \sqrt{2W})$  and  $(\sqrt{2W}, +\infty)$  and can be analytically continued into  $k_1$ -complex plane. We can see the problem in point  $+\sqrt{2W}$ , where locally we have square-root-like behaviour  $\sqrt{2W - k_1^2}$ , which brings the analytic continuation into two Riemann sheets. In other words, the point  $+\sqrt{2W}$  is the branch point and the analytically continued function will be multifunction (multi-valued function).

If we take the relation (3.9) as the definition of the analytic continuation and replace  $K_2$  with multifunction  $\mp\sqrt{2W - k_1^2}$ , this fulfills the Cauchy–Riemann conditions in whole  $k_1$ -complex plane (both sheets) except for zeroes of  $\Delta_+(k_1)$  (poles) and points  $\pm\sqrt{2W}$  (branch points).

The poles on the positive imaginary axis ( $\text{Re}(k_1) = 0, \text{Im}(k_1) > 0$ ) correspond to *bound states*, poles on the negative imaginary axis ( $\text{Re}(k_1) = 0, \text{Im}(k_1) < 0$ ) are called *virtual states* and the poles in The lower half-plane ( $\text{Re}(k_1) \neq 0, \text{Im}(k_1) < 0$ ) usually correspond to *resonances*.

From (3.9) we can see, that poles of the S matrix are zeroes of  $\Delta_+(k_1)$  (the sign  $\pm$  depends on the sheet)

$$\Delta_+(k_1) = (a - ik_1) \left( b \pm \sqrt{2W - k_1^2} \right) - |c|^2.$$

The condition for roots can be rewritten as

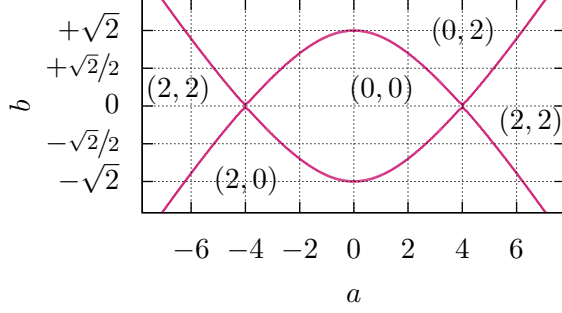
$$\Delta_+(k_1)(a, b, |c|) = 0 \iff \text{Re}(\Delta_+(k_1))(a, b, |c|) = 0 \wedge \text{Im}(\Delta_+(k_1))(a, b) = 0.$$

The condition  $\text{Im}(\Delta_+(k_1)) = 0$  is independent of the parameter  $|c|$ . We can plot the solution of the condition  $\text{Im}(\Delta_+(k_1)) = 0$  for fixed parameters  $a$  and  $b$  and plot the solution of the condition  $\text{Re}(\Delta_+(k_1)) = 0$  for various values of the parameter  $|c|$ . Intersections of the plotted curves are wanted poles of the S matrix. In the Figures from 3.6 to 3.12 in the upper halves we have plotted for various parameters  $a$  and  $b$  solutions of equation  $\text{Im}(\Delta_+(k_1)) = 0$  in two Riemann  $k_1$ -sheets and for given  $|c|$  (from 0 to 1.6 with step 0.1) the solutions of equation  $\text{Re}(\Delta_+(k_1)) = 0$ ; in the lower halves we have plotted scattering quantities (the scattering probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$ , the eigenphases  $\delta_i(k_1)$ ) to demonstrate their relation to poles of the S matrix.

#### 3.3.1 Phenomena

1. The dark green lines trace the movement of the poles with increasing parameter  $|c|$ . Their structure changes with parameters  $a$  and  $b$ : *no intersection point* (the left Riemann sheet of Figures from 3.6 to 3.9, the right Riemann sheet of all Figures from 3.6 to 3.12), *1 intersection point* (borderline case, the left Riemann sheet of Figure 3.10) and *2 intersection points* (the left Riemann sheet

<sup>10</sup>More precisely: If two analytic functions on some domain (simply connected open subset of the complex plane) are same on some line segment of the domain, they are same on the domain.



$$\begin{aligned}
& a^6 - 3a^4(b^2 + 10W) + \\
& + 3a^2(b^4 - 52b^2W + 64W^2) - \\
& - (b^2 - 2W)(b^2 + 16W)^2 = 0.
\end{aligned}
\tag{3.11}$$

**Figure 3.5:** The solution of the equation (3.11) and the number of intersection points on the first and the second Riemann sheet  $(N_1, N_2)$  in different regions divided by the solution.

of Figures 3.11 and 3.12). Further exploration uncovers that the borderline case of one intersection point happens for parameters  $a$  and  $b$  satisfying the equation (3.11).<sup>11,12</sup> The solution of such parameters  $a$  and  $b$  is plotted in Figure 3.5. The convex curve divides plane on the *no intersection point region* (above the curve) and the *2 intersection point region* (under the curve) on the first Riemann sheet. Similarly, the concave curve divides plane on the *2 intersection points region* (above the curve) and the *no intersection point region* (under the curve) on the second Riemann sheet.

2. We can see in the Figures from 3.6 to 3.9 that with increasing parameter  $|c|$  the *virtual state* becomes the *bound state*, which can be observed in the change of the limit eigenphase difference  $\delta_1(0) - \delta_1(+\infty)$  by value  $+\pi$ .<sup>13</sup>
3. The poles of the S matrix in the lower half-plane usually linked to resonances do correspond to resonant behaviour in scattering quantities (rapid changes, e.g. Figure from 3.8 to 3.11), but this model also provides counter-examples. For instance in Figure 3.12 the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  or the eigenphases  $\delta_i(k_1)$  do not have rapid changes or any other similarities with resonant behaviour. This usually happens to poles further from real axis.

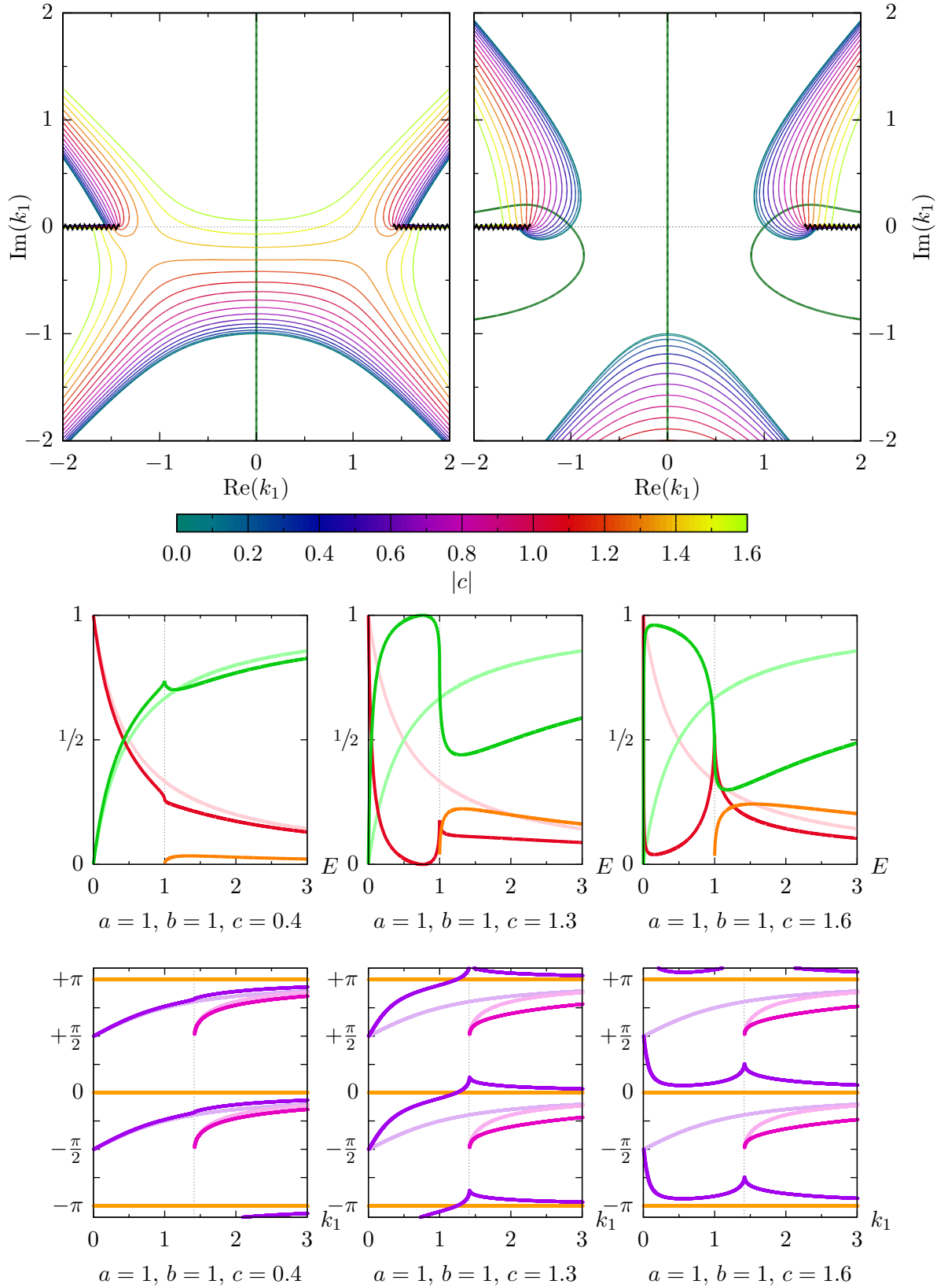
In the figure 3.6 for  $a = 1$  and  $b = 1$  we can see virtual state, which with increasing  $|c|$  becomes bound state.

<sup>11</sup>We note that, we have chosen threshold  $W = 1$  and the parameter  $W$  is redundant. We can always rescale:  $W \rightarrow 1$ ,  $E \rightarrow \frac{E}{W}$ ,  $x \rightarrow \frac{x}{\sqrt{W}}$ ,  $a \rightarrow \frac{a}{\sqrt{W}}$ ,  $b \rightarrow \frac{b}{\sqrt{W}}$  and  $c \rightarrow \frac{c}{\sqrt{W}}$ .

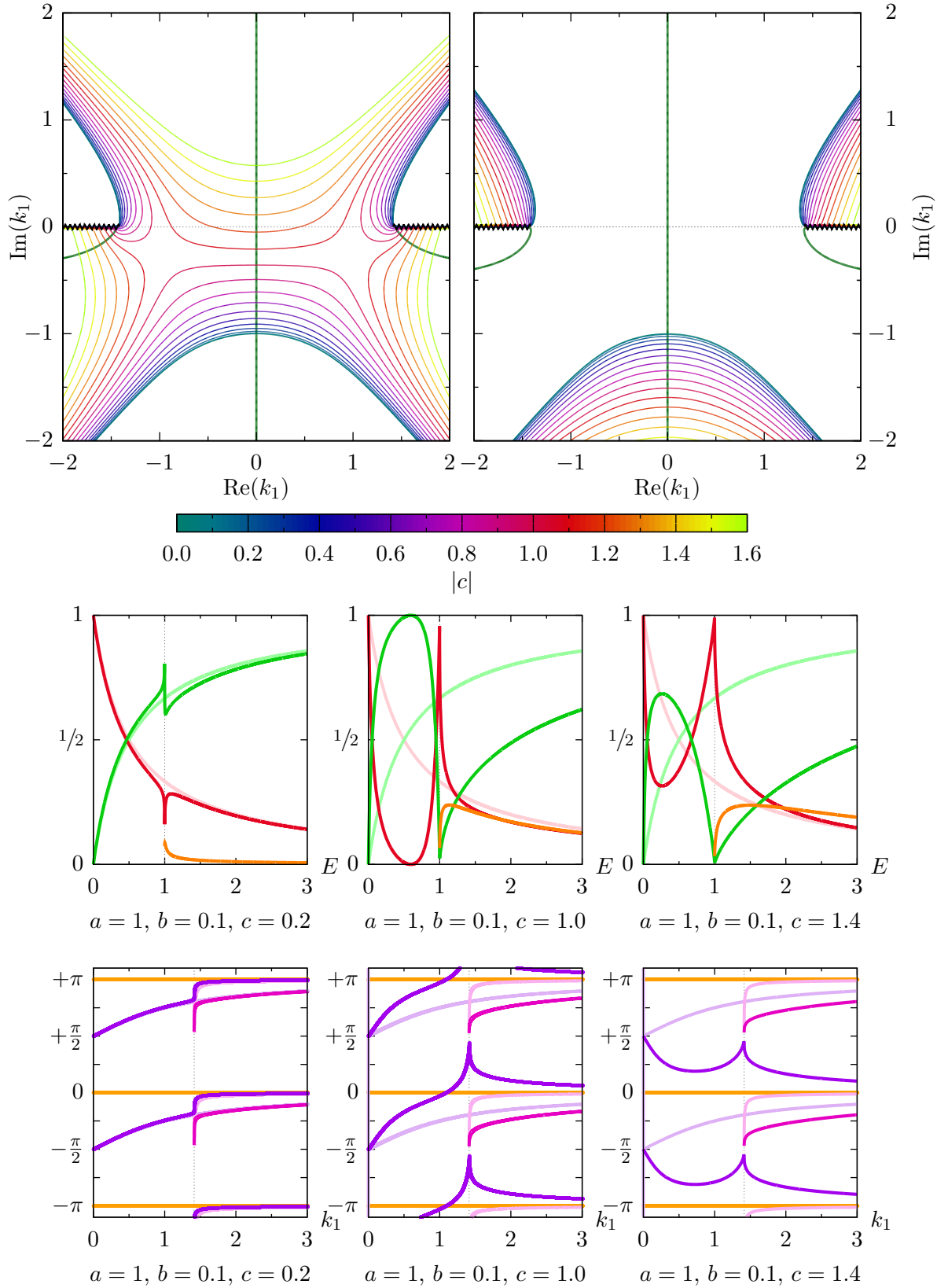
<sup>12</sup>The solution for  $a = 1$  is  $b = \pm \sqrt{-9 - 3 \times 2^{\frac{2}{3}}(-11 + 5\sqrt{5})^{\frac{1}{3}} + 3 \times 2^{\frac{2}{3}}(11 + 5\sqrt{5})^{\frac{1}{3}}} \approx \pm 1.29989$ , which is in a good agreement with the chosen value  $c = -1.3$  in Figure 3.10.

<sup>13</sup>This can be understood in analogy to one-channel case as the implication of *Levinson's theorem* (for instance Taylor (2006), p. 227 [6]). When the virtual state becomes the bound state, then the difference  $\delta(0) - \delta(+\infty)$  changes by constant  $+\pi$ . However for proper interpretation (explaining discrepancies like "why this happens only for some eigenphases", "meaning of the number  $n_0$ " and so on) we would need the generalized Levinson's theorem for the multichannel scattering. This is beyond the scope of this footnote, this thesis and maybe even the universe itself.

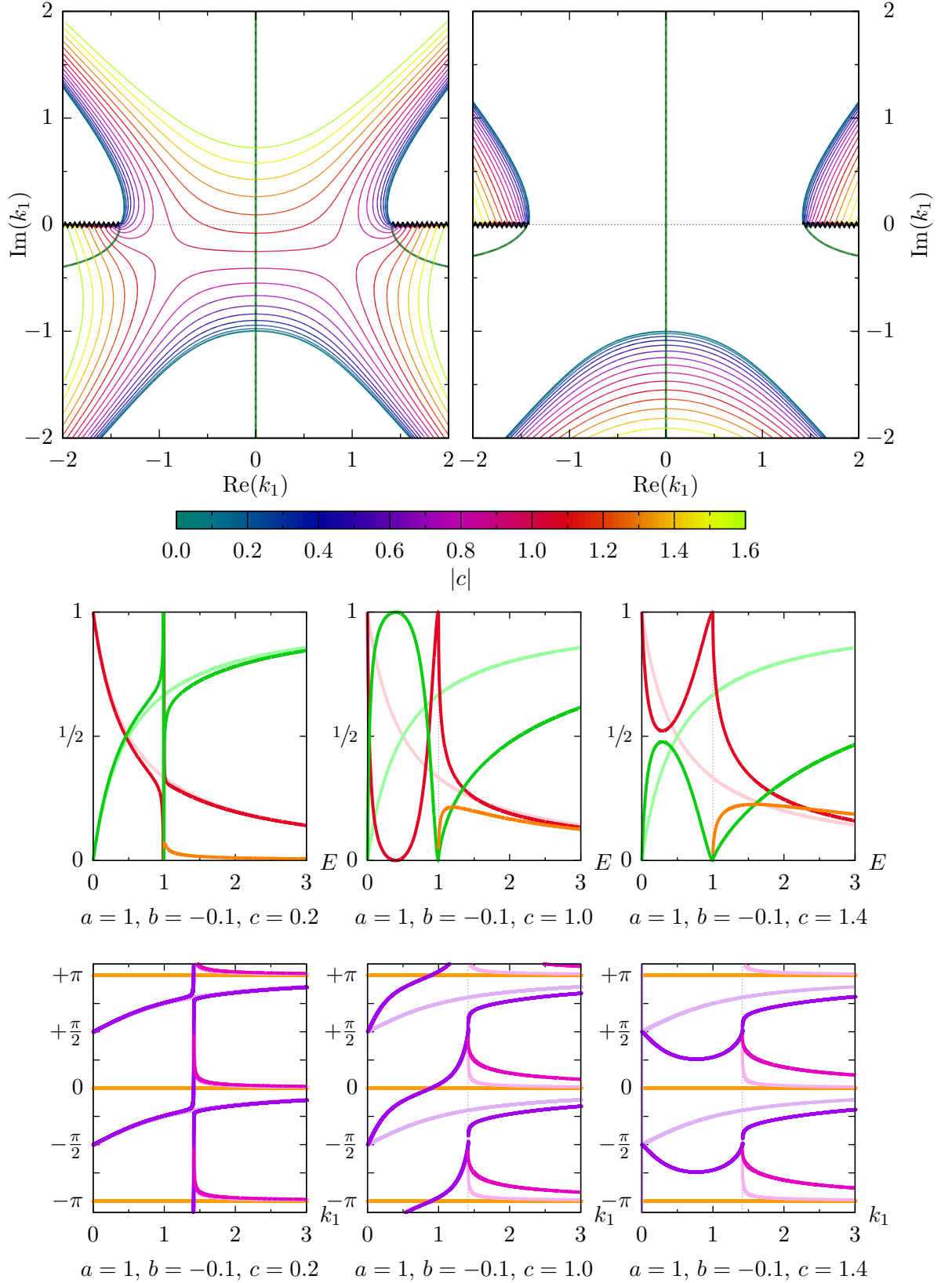




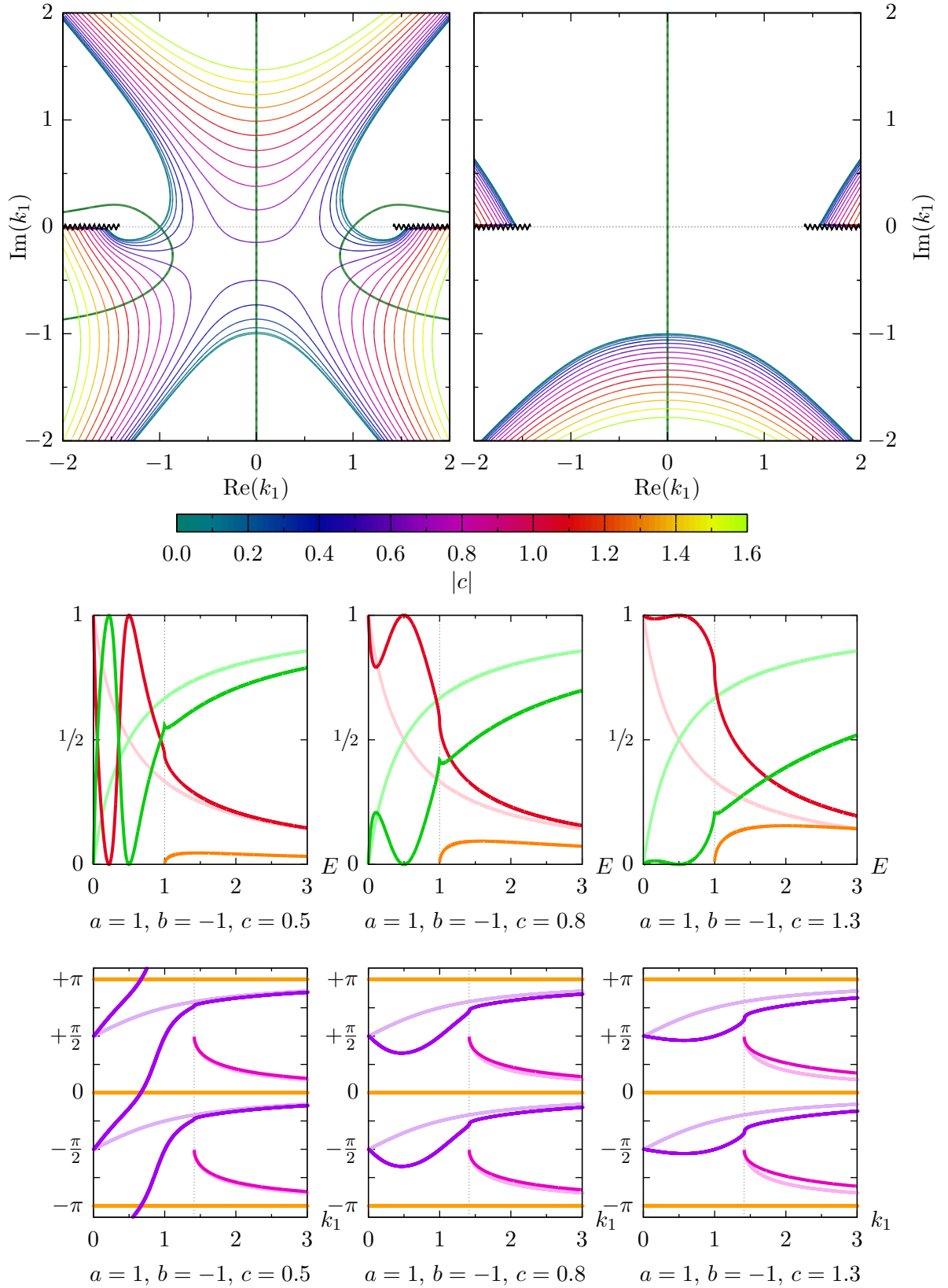
**Figure 3.6:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = 1$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



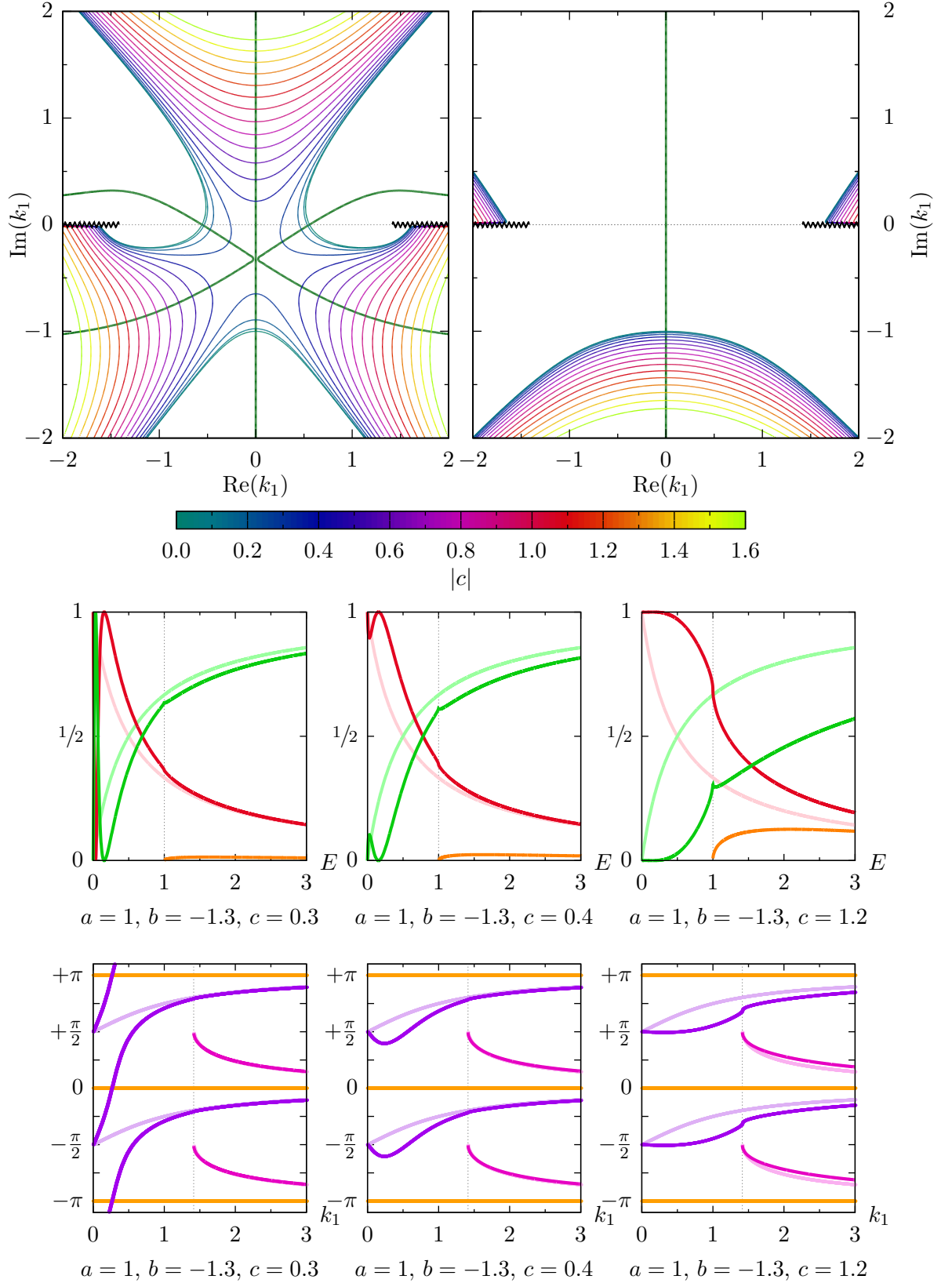
**Figure 3.7:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = 0.1$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



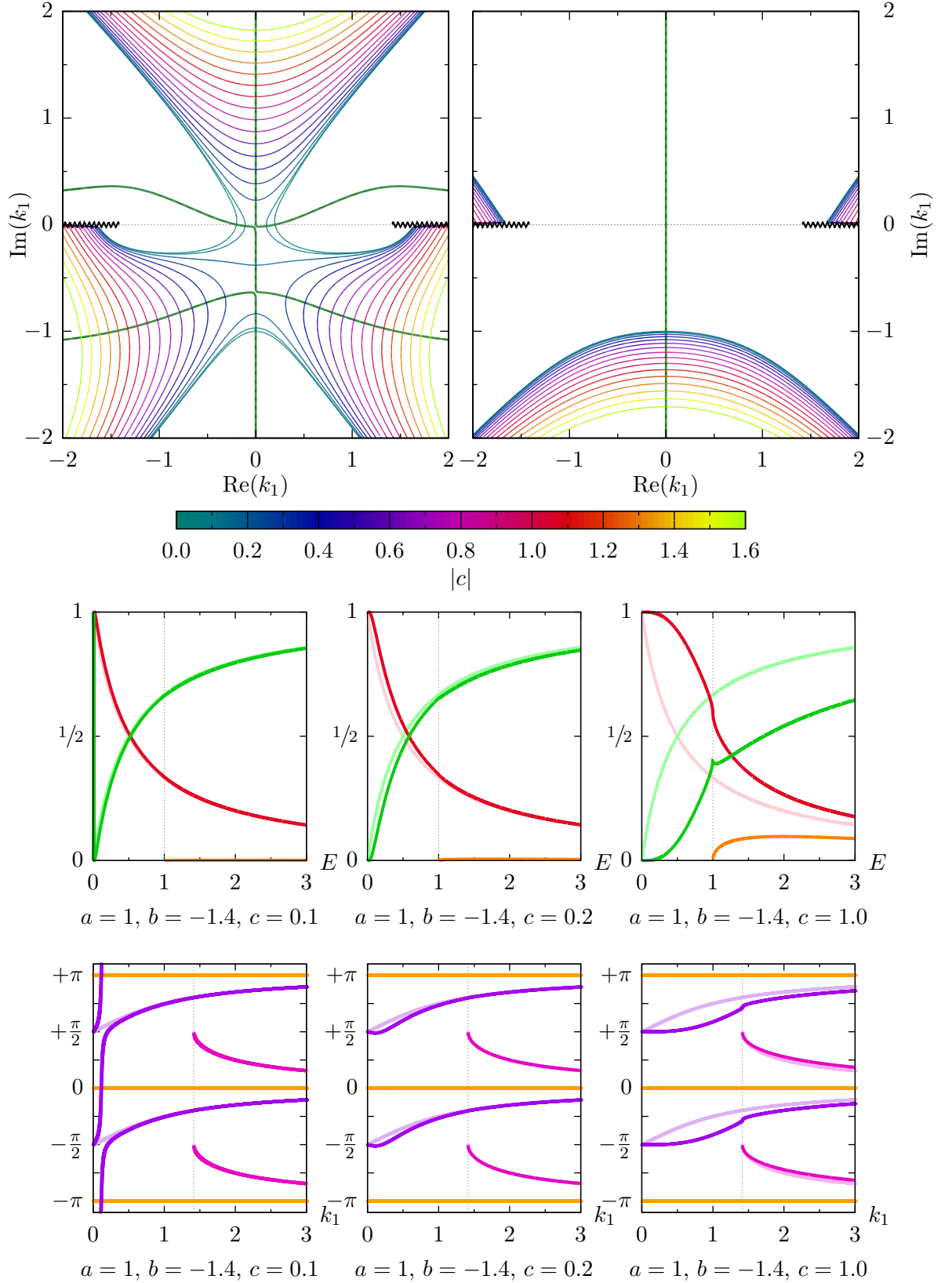
**Figure 3.8:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = -0.1$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



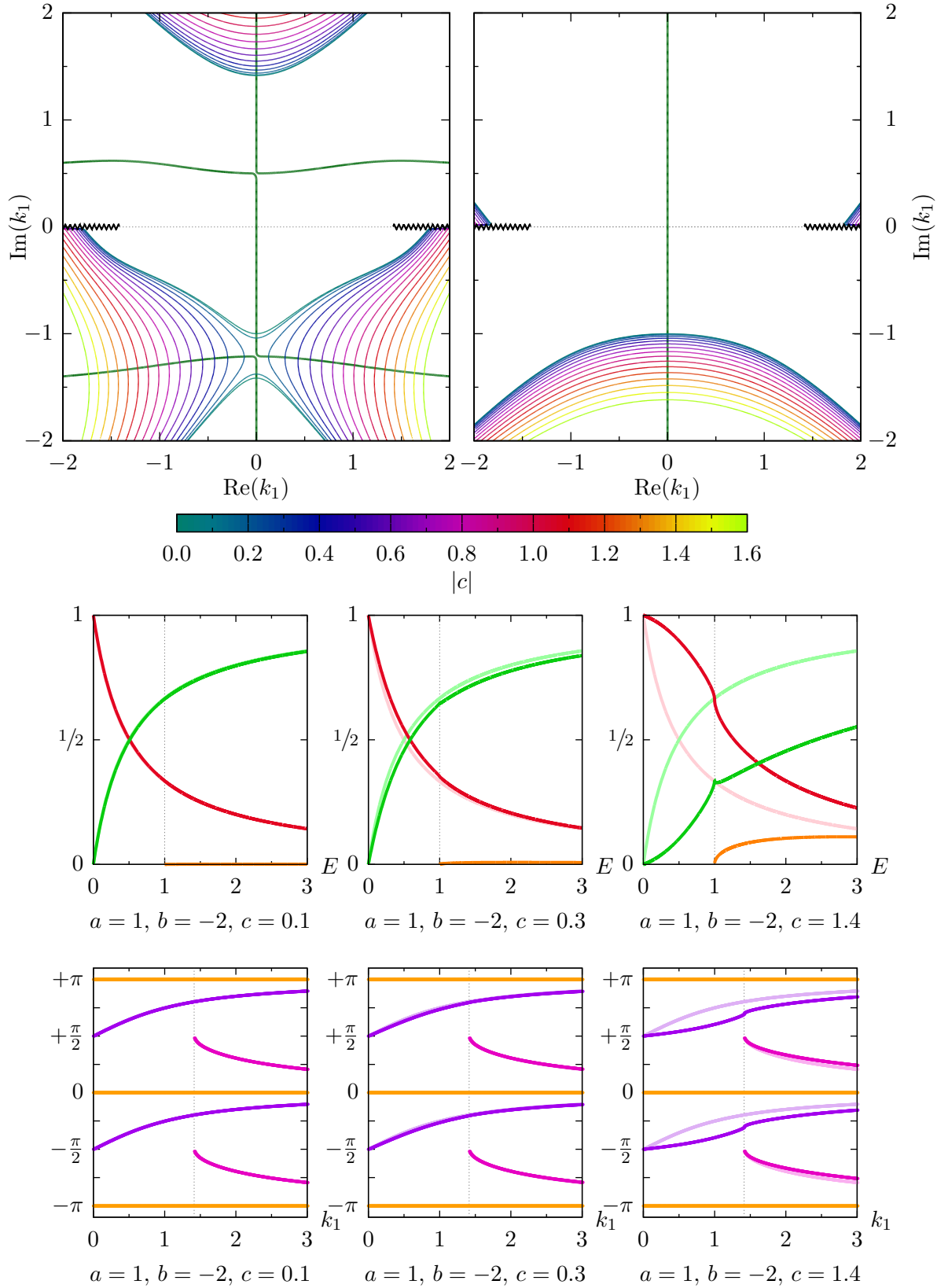
**Figure 3.9:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = -1$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



**Figure 3.10:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = -1.3$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



**Figure 3.11:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = -1.4$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.



**Figure 3.12:** The upper half: Solutions of  $\text{Im}(\Delta_+(k_1)) = 0$  (dark green bold lines) and  $\text{Re}(\Delta_+(k_1)) = 0$  (coloured lines, parameter  $|c|$  from 0 to 1.6 with step 0.1) on two Riemann sheets for  $a = 1$  and  $b = -2$ . The lower half: The energy dependence of the probabilities  $T_{n'1}(E)$  and  $R_{n'1}(E)$  and  $k_1$ -dependence of the eigenphases  $\delta_i(k_1)$  for various settings of parameters.

# 4. Theoretical description of resonances

In this chapter we will apply projection methods to separate the *resonant scattering* (sharp, rapid energy dependence) and the *background scattering* (smooth energy dependence) in scattering quantities, namely T matrix. Resonances (in this approach) are naturally understood as the effect of the interaction between the *continuum of open channel(s)* and *quasi-bound state(s) of closed channel(s)*.<sup>1</sup> First, we will develop brief insight to the theory, then we will use formalism to our model.

## 4.1 Projection-operator formalism

As mentioned before, near the resonance energy the particle is trapped into unstable quasi-bound state (of a closed channel) and subsequently released. The mechanism causes the rapid changes of cross sections in energy dependence. This leads us to the idea of separation the Hilbert space  $\mathcal{H}$  into the space of quasi-states  $\mathcal{Q}$  and remaining space of non-resonant continuum  $\mathcal{P}$ .

$$\mathcal{H} = \mathcal{P} \oplus \mathcal{Q}$$

To achieve the separation of vectors and operators according to these subspaces, we introduce (orthogonal) *projection operators*  $\hat{P}$  and  $\hat{Q}$  projecting onto the subspace  $\mathcal{P}$  and  $\mathcal{Q}$  respectively.

$$\begin{aligned} \hat{P} : \mathcal{H} &\rightarrow \mathcal{P} & \hat{Q} : \mathcal{H} &\rightarrow \mathcal{Q} & \hat{P} + \hat{Q} &= \hat{1} \\ \hat{P}^2 &= \hat{P} & \hat{P}^+ &= \hat{P} & \hat{Q}^2 &= \hat{Q} & \hat{Q}^+ &= \hat{Q} & \hat{P}\hat{Q} &= \hat{Q}\hat{P} = 0 \end{aligned}$$

We recall the splitting of the full Hamiltonian  $\hat{H}$  into free Hamiltonian  $\hat{H}_0$  and potential  $\hat{V}$  (1.4) and corresponding *Lippmann-Schwinger equation for  $|\mathbf{p}\pm\rangle$*  (1.25).

$$\hat{H} = \underbrace{\hat{H}_0}_{\hat{T}} + \hat{V} \quad |\mathbf{p}\pm\rangle = |\mathbf{p}\rangle + \hat{G}_0(E_p \pm i0)\hat{V}|\mathbf{p}\pm\rangle$$

In the same fashion we can do for Hamiltonians  $\hat{T}_{PP}^2$ ,  $\hat{H}_{PP}$  and  $\hat{H}$ .<sup>3</sup>

$$\hat{T}_{PP} = \hat{T} + (\hat{T}_{PP} - \hat{T}) \quad |\mathbf{p}_0^{\mathcal{P}}\pm\rangle = |\mathbf{p}\rangle + \hat{G}_0(E_p \pm i0)(\hat{T}_{PP} - \hat{T})|\mathbf{p}_0^{\mathcal{P}}\pm\rangle \quad (4.1)$$

$$\hat{H}_{PP} = \hat{T}_{PP} + (\hat{H}_{PP} - \hat{T}_{PP}) \quad |\mathbf{p}^{\mathcal{P}}\pm\rangle = |\mathbf{p}_0^{\mathcal{P}}\pm\rangle + \hat{G}_0^{\mathcal{P}}(E_p \pm i0)(\hat{H}_{PP} - \hat{T}_{PP})|\mathbf{p}^{\mathcal{P}}\pm\rangle \quad (4.2)$$

$$\hat{H} = \hat{H}_{PP} + (\hat{H} - \hat{H}_{PP}) \quad |\mathbf{p}\pm\rangle = |\mathbf{p}^{\mathcal{P}}\pm\rangle + \hat{G}^{\mathcal{P}}(E_p \pm i0)(\hat{H} - \hat{H}_{PP})|\mathbf{p}\pm\rangle \quad (4.3)$$

<sup>1</sup>One could understand the approach as a strict mathematical technique without any physical weight, but for the key element (the choice of the quasi-bound state(s) space  $\mathcal{Q}$ ) there is no mathematical formalism, only physical intuition. Incorrect choice could add false resonance peaks in background and resonant part. On the other hand, we should point out, that only rough estimate is necessary, because the small errors are corrected within the formalism.

<sup>2</sup>We introduce the notation  $\hat{A}_{XY} := \hat{X}\hat{A}\hat{Y}$ .

<sup>3</sup>This is justified only for potentials satisfying the asymptotic condition. The potential  $(\hat{H}_{PP} - \hat{T}_{PP}) = \hat{V}_{PP}$  is full potential  $\hat{V}$  (for which we assume, that the asymptotic condition is fulfilled) restricted onto subspace  $\mathcal{P}$ , thus condition is fulfilled. For potentials  $(\hat{T}_{PP} - \hat{T}) = -\hat{T}_{1Q} - \hat{T}_{Q1} + \hat{T}_{QQ}$  and  $(\hat{H} - \hat{H}_{PP}) = \hat{H}_{1Q} + \hat{H}_{Q1} - \hat{H}_{QQ}$  and for the subspace  $\mathcal{Q}$  equal to the linear span of finite number of quasi-bound states (square-integrable functions) the asymptotic condition is also fulfilled.



The vectors  $|\mathbf{p}\rangle$ ,  $|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$ ,  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$  and  $|\mathbf{p}\pm\rangle$  are improper eigenvectors (asymptotes) of Hamiltonians  $\hat{T}$ ,  $\hat{T}_{PP}$ ,  $\hat{H}_{PP}$  and  $\hat{H}$  respectively. Therefore the vectors  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$  represent the non-resonant continuum. Similarly, the operators  $\hat{G}_0(z)$ ,  $\hat{G}_0^{\mathcal{P}}(z)$ ,  $\hat{G}^{\mathcal{P}}(z)$  and  $\hat{G}(z)$  are Green's operators of Hamiltonians  $\hat{T}$ ,  $\hat{T}_{PP}$ ,  $\hat{H}_{PP}$  and  $\hat{H}$  respectively. It can be shown that the vectors  $|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$  and  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$  are orthogonal to subspace  $\mathcal{Q}^4$

$$\hat{Q}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = \hat{Q}|\mathbf{p}^{\mathcal{P}\pm}\rangle = 0 \implies \hat{P}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = |\mathbf{p}_0^{\mathcal{P}\pm}\rangle, \quad \hat{P}|\mathbf{p}^{\mathcal{P}\pm}\rangle = |\mathbf{p}^{\mathcal{P}\pm}\rangle.$$

Using *two-potential formula*<sup>5</sup> twice we can separate the on-shell T matrix  $t(\mathbf{p}' \leftarrow \mathbf{p})$  into three terms

$$\begin{aligned} t(\mathbf{p}' \leftarrow \mathbf{p}) &= \underbrace{\langle \mathbf{p}' | \hat{H}_{PP} - \hat{T} | \mathbf{p}^{\mathcal{P}+} \rangle}_{=: t_{\text{bg}}(\mathbf{p}' \leftarrow \mathbf{p})} + \underbrace{\langle \mathbf{p}'^{\mathcal{P}-} | \hat{H} - \hat{H}_{PP} | \mathbf{p}+ \rangle}_{=: t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})} \\ &= \underbrace{\langle \mathbf{p}' | \hat{T}_{PP} - \hat{T} | \mathbf{p}_0^{\mathcal{P}+} \rangle}_{=: t_{\text{ortho}}(\mathbf{p}' \leftarrow \mathbf{p})} + \underbrace{\langle \mathbf{p}_0^{\mathcal{P}-} | \hat{H}_{PP} - \hat{T}_{PP} | \mathbf{p}^{\mathcal{P}+} \rangle}_{=: t_{\text{dir}}(\mathbf{p}' \leftarrow \mathbf{p})} + \langle \mathbf{p}'^{\mathcal{P}-} | \hat{H} - \hat{H}_{PP} | \mathbf{p}+ \rangle. \end{aligned}$$

Because the vectors  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$  represent the non-resonant continuum, the first term is often referred to as *background scattering*  $t_{\text{bg}}(\mathbf{p}' \leftarrow \mathbf{p})$ , which implies that the remaining term is responsible for *resonant scattering*  $t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})$ . The background term can be split into two terms usually called *orthogonality scattering*<sup>6</sup>  $t_{\text{ortho}}(\mathbf{p}' \leftarrow \mathbf{p})$  and *direct scattering*<sup>7</sup>  $t_{\text{dir}}(\mathbf{p}' \leftarrow \mathbf{p})$ . Usually one needs only separation into two terms: the background (non-resonant) and the resonant term.

First, to achieve this separation, we choose the subspace  $\mathcal{Q}$  as linear span of  $M$  orthonormal proper vectors  $\{|\chi_n\rangle\}_{n=1}^M$ . From the theory of spectral decomposition the eigenvectors of the Hamiltonian  $\hat{H}$ : *proper vectors*  $|n\rangle$  (the bound states from subspace  $\mathcal{B}$ ) and *improper vectors*  $|\mathbf{p}\pm\rangle$  (the scattering states from subspace  $\mathcal{R}$ ), form the orthonormal basis.

$$\begin{aligned} \mathcal{H} &= \mathcal{B} \oplus \mathcal{R} \\ \langle n' | n \rangle &= \delta_{n'n} \\ \langle \mathbf{k}' \pm | \mathbf{k} \pm \rangle &= \delta_N(\mathbf{k}' - \mathbf{k}) \\ \langle n | \mathbf{k} \pm \rangle &= 0 \end{aligned} \quad \hat{1} = \underbrace{\sum_n |n\rangle \langle n|}_{\hat{1}_{\mathcal{B}}} + \underbrace{\int_{\mathbb{R}^N} d\mathbf{k} |\mathbf{k}\pm\rangle \langle \mathbf{k}\pm|}_{\hat{1}_{\mathcal{R}}}$$

In the same fashion, we can write for the subspaces  $\mathcal{Q}$  and  $\mathcal{P}$ .

$$\begin{aligned} \mathcal{H} &= \mathcal{Q} \oplus \mathcal{P} \\ \langle \chi_{n'} | \chi_n \rangle &= \delta_{n'n} \\ \langle \mathbf{k}'^{\mathcal{P}\pm} | \mathbf{k}^{\mathcal{P}\pm} \rangle &= \delta_N(\mathbf{k}' - \mathbf{k}) \\ \langle \chi_n | \mathbf{k}^{\mathcal{P}\pm} \rangle &= 0 \end{aligned} \quad \hat{1} = \underbrace{\sum_{n=1}^M |\chi_n\rangle \langle \chi_n|}_{\hat{1}_{\mathcal{Q}} = \hat{Q}} + \underbrace{\int_{\mathbb{R}^N} d\mathbf{k} |\mathbf{k}^{\mathcal{P}\pm}\rangle \langle \mathbf{k}^{\mathcal{P}\pm}|}_{\hat{1}_{\mathcal{P}} = \hat{P}}$$

<sup>4</sup>For the vector  $|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$  as eigenvector we can write

$$E\hat{Q}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = \hat{Q}E|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = \hat{Q}\hat{T}_{PP}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = \underbrace{\hat{Q}\hat{P}}_0 \hat{T}\hat{P}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = 0.$$

Similarly we can write for  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$ .

<sup>5</sup>*Two-potential formula.* (Taylor (2006), p. 270-271 [6]) If the full potential  $\hat{V}$  is equal to sum of two potentials  $\hat{V} = \hat{V}_1 + \hat{V}_2$ , then we can write for the on-shell T matrix  $t(\mathbf{p}' \leftarrow \mathbf{p})$

$$t(\mathbf{p}' \leftarrow \mathbf{p}) = \langle \mathbf{p}' | \hat{V}_1 | \mathbf{p}^1+ \rangle + \langle \mathbf{p}'^1- | \hat{V}_2 | \mathbf{p}+ \rangle,$$

where  $|\mathbf{p}^1\pm\rangle$  are improper eigenvectors of Hamiltonian  $\hat{H}_0 + \hat{V}_1$  (i.e. the solutions of Lippmann-Schwinger equation).

<sup>6</sup>Coming from orthogonal separation of asymptote space  $\mathcal{H}$  into  $\mathcal{P}$  and  $\mathcal{Q}$ .

<sup>7</sup>As direct scattering without any trapping into quasi-bound states.

### 4.1.1 Orthogonal scattering

As shown in Domcke's article (1983) [3], it is possible to solve<sup>8</sup> the orthogonal scattering in closed form. We start with Lippmann-Schwinger equation for  $|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$  (4.1) with the potential  $(\hat{T}_{PP} - \hat{T}) = -\hat{T}_{IQ} - \hat{T}_{QI} + \hat{T}_{QQ}$  and using  $\hat{Q}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = 0$  we get

$$\begin{aligned} |\mathbf{p}_0^{\mathcal{P}\pm}\rangle &= |\mathbf{p}\rangle + \hat{G}_0(E_p \pm i0)(-\hat{T}_{IQ} - \hat{T}_{QI} + \hat{T}_{QQ})|\mathbf{p}_0^{\mathcal{P}\pm}\rangle \\ &= |\mathbf{p}\rangle - \sum_{n=1}^M \hat{G}_0(E_p \pm i0)|\chi_n\rangle\langle\chi_n|\hat{T}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle. \end{aligned}$$

The solution is obtained in closed form<sup>9</sup>

$$|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = |\mathbf{p}\rangle - \sum_{\substack{n=1 \\ m=1}}^M \hat{G}_0(E_p \pm i0)|\chi_n\rangle A(E_p \pm i0)_{nm}^{-1} \langle\chi_m|\mathbf{p}\rangle, \quad (4.4)$$

where  $A(z)^{-1}$  is inverted  $M \times M$  matrix of  $M \times M$  matrix  $A(z)$  defined as  $A(z)_{nm} := \langle\chi_n|\hat{G}_0(z)|\chi_m\rangle$ . Using the same steps with the on-shell T matrix  $t_{\text{ortho}}(\mathbf{p}' \leftarrow \mathbf{p})$  and closed form of  $\langle\chi_n|\hat{T}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$  we get

$$t_{\text{ortho}}(\mathbf{p}' \leftarrow \mathbf{p}) = - \sum_{\substack{n=1 \\ m=1}}^M \langle\mathbf{p}'|\chi_n\rangle A(E_p + i0)_{nm}^{-1} \langle\chi_m|\mathbf{p}\rangle. \quad (4.5)$$

In same fashion the free Green's operator  $\hat{G}_{0,PP}^{\mathcal{P}}(z)$  in subspace  $\mathcal{P}$  is obtained

$$\hat{G}_{0,PP}^{\mathcal{P}}(z) = \hat{G}_0(z) - \sum_{\substack{n=1 \\ m=1}}^M \hat{G}_0(z)|\chi_n\rangle A(z)_{nm}^{-1} \langle\chi_m|\hat{G}_0(z). \quad (4.6)$$

The off-diagonal terms  $\hat{G}_{0,PQ}^{\mathcal{P}}(z)$  and  $\hat{G}_{0,QP}^{\mathcal{P}}(z)$  are from definition zero and the free Green's operator  $\hat{G}_{0,QQ}^{\mathcal{P}}(z)$  in subspace  $\mathcal{Q}$  is simply  $z^{-1}\hat{Q}$ .

### 4.1.2 Resonant scattering

It is possible to express the resonant scattering T matrix  $t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})$  without using full scattering continuum  $|\mathbf{p}\pm\rangle$  and instead to use background scattering continuum  $|\mathbf{p}^{\mathcal{P}\pm}\rangle$  (e.g. in [2]). From the definition of the resonant scattering T matrix  $t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})$  for the potential  $(\hat{H} - \hat{H}_{PP}) = \hat{H}_{QQ} + \hat{H}_{QP} + \hat{H}_{PQ}$  and using  $\hat{Q}|\mathbf{p}^{\mathcal{P}\pm}\rangle = 0$  we get

$$t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p}) = \langle\mathbf{p}'^{\mathcal{P}}|-\hat{H}_{QQ} + \hat{H}_{QP} + \hat{H}_{PQ}|\mathbf{p}\rangle = \langle\mathbf{p}'^{\mathcal{P}}|-\hat{P}\hat{H}\hat{Q}|\mathbf{p}\rangle.$$

In order to get rid of the term  $\hat{Q}|\mathbf{p}\rangle$ , we will project the Lippmann-Schwinger equation for  $|\mathbf{p}\pm\rangle$  (4.3) into subspaces  $\mathcal{P}$  and  $\mathcal{Q}$

$$\hat{P}|\mathbf{p}\pm\rangle = \underbrace{\hat{P}|\mathbf{p}^{\mathcal{P}\pm}\rangle}_{|\mathbf{p}^{\mathcal{P}\pm}\rangle} + \hat{P}\hat{G}^{\mathcal{P}}(E_p \pm i0)(\hat{H}_{QQ} + \hat{H}_{QP} + \hat{H}_{PQ})|\mathbf{p}\pm\rangle, \quad (4.7)$$

$$\hat{Q}|\mathbf{p}\pm\rangle = \underbrace{\hat{Q}|\mathbf{p}^{\mathcal{P}\pm}\rangle}_0 + \underbrace{\hat{Q}\hat{G}^{\mathcal{P}}(E_p \pm i0)}_{(E_p \pm i0)^{-1}}(\hat{H}_{QQ} + \hat{H}_{QP} + \hat{H}_{PQ})|\mathbf{p}\pm\rangle, \quad (4.8)$$

<sup>8</sup>To find the scattering vectors  $|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$ , on-shell T matrix  $t_{\text{ortho}}(\mathbf{p}' \leftarrow \mathbf{p})$  and the Green's operator  $\hat{G}_0^{\mathcal{P}}(z)$ .

<sup>9</sup>After acting with  $\langle\chi_i|\hat{T}$  from the left on the equation we get solvable matrix equation for  $\langle\chi_n|\hat{T}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle$

$$\sum_{m=1}^M \underbrace{\langle\chi_k|\hat{G}_0(E_p \pm i0)|\chi_m\rangle}_{A_{km}(E_p \pm i0)} \langle\chi_m|\hat{T}|\mathbf{p}_0^{\mathcal{P}\pm}\rangle = \langle\chi_k|\mathbf{p}\rangle.$$

where we used fact, that the Green's operator  $\widehat{G}^{\mathcal{P}}(z)$  is diagonal with respect to subspaces  $\mathcal{P}$  and  $\mathcal{Q}$ , therefore  $\widehat{G}_{PQ}^{\mathcal{P}}(z) = \widehat{G}_{QP}^{\mathcal{P}}(z) = 0$  and  $\widehat{G}_{QQ}^{\mathcal{P}}(z) = z^{-1}\widehat{Q}$ . We substitute in the second equation (4.8) the term  $\widehat{P}|\mathbf{p}\pm\rangle$  from the first equation (4.7) and we get equation for  $\widehat{Q}|\mathbf{p}\pm\rangle$  with the solution

$$\widehat{Q}|\mathbf{p}\pm\rangle = \left[ (E_p \pm i0) - \widehat{H}_{QQ} - \widehat{H}_{QP}\widehat{G}^{\mathcal{P}}(E_p \pm i0)\widehat{H}_{PQ} \right]^{-1} \widehat{H}_{QP}|\mathbf{p}^{\mathcal{P}}\pm\rangle.$$

Using this result we can write the resonant scattering T matrix  $t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})$  as

$$t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p}) = \langle \mathbf{p}'^{\mathcal{P}} | \widehat{H}_{PQ} \left[ (E_p + i0) - \widehat{H}_{QQ} - \widehat{H}_{QP}\widehat{G}^{\mathcal{P}}(E_p + i0)\widehat{H}_{PQ} \right]^{-1} \widehat{H}_{QP} | \mathbf{p}^{\mathcal{P}+} \rangle. \quad (4.9)$$

Even though this formula looks horribly clumsy, it can be broken down into three matrix element evaluated on subspace  $\mathcal{Q}$ . We define the *discrete states' Hamiltonian*  $H_{mn}$ , *discrete-states-continuum coupling*  $V_{m,\mathbf{p}}^{\pm}$  and complex *level-shift matrix*  $F_{mn}(z)$  as

$$\begin{aligned} H_{mn} &:= \langle \chi_m | \widehat{H} | \chi_n \rangle, \\ V_{m,\mathbf{p}}^{\pm} &:= \langle \chi_m | \widehat{H} | \mathbf{p}^{\mathcal{P}}\pm \rangle, \\ F_{mn}(z) &:= \langle \chi_m | \widehat{H} \widehat{G}_{PP}^{\mathcal{P}}(z) \widehat{H} | \chi_n \rangle =: \Delta_{mn}(z) - \frac{i}{2} \Gamma_{mn}(z), \end{aligned}$$

where  $\Delta_{mn}(z)$  is real part of level-shift matrix  $F_{mn}(z)$  and  $\Gamma_{mn}(z)$  is (up to multiplicative constant  $-1/2$ ) imaginary part of level-shift matrix also called *width*<sup>10</sup>.

Applying the formalism for subspace  $\mathcal{Q}$  of one normalised discrete state  $|\chi_1\rangle$  simplifies the inverse of a  $M \times M$  matrix in (4.9) to inverse of a number and we get

$$t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p}) = \frac{(V_{1,\mathbf{p}'}^-)^* V_{1,\mathbf{p}}^+}{E - H_{11} - F_{11}(E_p + i0)} = \frac{(V_{1,\mathbf{p}'}^-)^* V_{1,\mathbf{p}}^+}{[E - H_{11} - \Delta_{11}(E_p + i0)] + \frac{i}{2} \Gamma_{11}(E_p + i0)}. \quad (4.10)$$

If the resonance is sharp, then the energy dependence of functions  $V_{1,\mathbf{p}}^{\pm}$ ,  $\Delta_{11}$  and  $\Gamma_{11}$  is negligible and we have obtained *Breit-Wigner resonance formula* with the resonance energy  $E_r = H_{11} + \Delta_{11}$  (the position of the peak in energy spectrum) and the resonance width  $\Gamma = \Gamma_{11}$  (the full width at half maximum of the peak).

## 4.2 Application of formalism

Now we will apply developed formalism to our model in regime of narrow resonance ( $b < 0$  and  $|b| \gg |c|$ ). *Explanation at the level of physical intuition:* In the case of no coupling between channels ( $|c| = 0$ ) the channels are isolated and cannot influence each other. If  $b < 0$ , there is bound state in the second channel (as seen in subsection 2.1.2) with the wave function

$$\langle x | \psi \rangle = \sqrt{-b} e^{b|x|} \hat{e}_2 \quad (4.11)$$

and the energy

$$E_{\text{bound}} = W - \frac{b^2}{2}. \quad (4.12)$$

Now we do small perturbation, we allow coupling  $|b| \gg |c| > 0$ . For energies  $W > E \geq 0$  the first channel is opened and the second one is closed. The bound state in the second channel will become quasi-bound state. This gives us second restriction

<sup>10</sup>The origin of the term and reason of the factor  $-1/2$  become obvious later, when we will show connection to Breit-Wigner resonance formula.

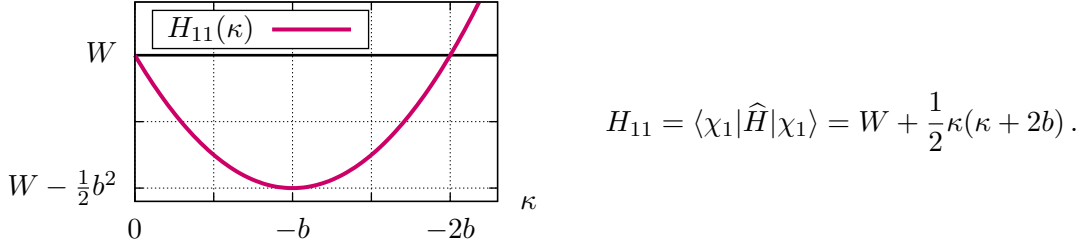
$-\sqrt{2W} < b < 0$ , otherwise the bound state of the unperturbed Hamiltonian would stay the bound state of the full Hamiltonian.

After this analysis the choice of subspace  $\mathcal{Q}$  becomes quite straightforward: linear span of  $M = 1$  normalized vector  $|\chi_1\rangle$

$$\langle x|\chi_1\rangle = \sqrt{\kappa}e^{-\kappa|x|}\hat{e}_2, \quad (4.13)$$

where  $\kappa > 0$  is parameter, ideally  $\kappa = -b$ . Later on we can test, how the choice of parameter  $\kappa$  (and consequently the choice of subspace  $\mathcal{Q}$ ) can affect the separation of on-shell T matrix  $t(\mathbf{p}' \leftarrow \mathbf{p})$ .

We have calculated the energy of the state  $|\chi_1\rangle$  in the full Hamiltonian  $\hat{H}$  (equation (A.14)) and plotted its  $\kappa$ -dependence in Figure 4.1. We can notice that the energy  $H_{11}$  will be same for the full Hamiltonian  $\hat{H}$  restricted only to the second channel. The state  $|\psi\rangle$  from equation (4.11) is the ground state of this restricted Hamiltonian with energy  $E_{\text{bound}}$  – equation (4.12). From the *variational principle* we know that the energy  $H_{11}$  of the state  $|\chi_1\rangle$  is always greater or equal than the energy of the ground state  $E_{\text{bound}}$  with equality for  $\kappa = -b$  (Figure 4.1).



**Figure 4.1:** The  $\kappa$ -dependence of energy  $H_{11}$  of the discrete state  $|\chi_1\rangle$  with marked threshold energy  $W$  (black line).

### 4.2.1 Orthogonal scattering

The orthogonal scattering have been solved in closed form. We only need to calculate for chosen subspace  $\mathcal{Q}$  three matrix elements  $\langle \chi_1 | k_n, s, n \rangle$ ,  $\langle x | \hat{G}_0(E \pm i0) | \chi_1 \rangle$  and  $\langle \chi_1 | \hat{G}_0(E \pm i0) | \chi_1 \rangle$  (Appendix A.2.1) and insert expressions into equations (4.4), (4.5) and (4.6) (for  $z = E \pm i0$ ).

$$\begin{aligned} \langle x | (k_n, s, n)_0^{\mathcal{P}} \pm \rangle &= \langle x | k_n, s, n \rangle - \frac{\langle x | \hat{G}_0(E \pm i0) | \chi_1 \rangle \langle \chi_1 | k_n, s, n \rangle}{\langle \chi_1 | \hat{G}_0(E \pm i0) | \chi_1 \rangle} \quad (3.2)(\text{A.11}) \\ &= \frac{\hat{e}_n}{\sqrt{2\pi}} e^{isk_n x} - \delta_{2n} \frac{\hat{e}_2}{\sqrt{2\pi}} \frac{2\kappa^2}{(2\kappa \mp ik_2)(\kappa \pm ik_2)^2} \left( \kappa e^{\pm ik_2|x|} \pm ik_2 e^{-\kappa|x|} \right) \quad (4.14) \end{aligned}$$

$$\begin{aligned} t_{\text{ortho}}(k_{n'}, s', n'; k_n, s, n) &= - \frac{\langle k_{n'}, s', n' | \chi_1 \rangle \langle \chi_1 | k_n, s, n \rangle}{\langle \chi_1 | \hat{G}_0(E + i0) | \chi_1 \rangle} \quad (\text{A.10}) \\ &= - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \frac{ik_2 \kappa^3}{\pi(2\kappa - ik_2)(\kappa + ik_2)^2}, \quad (\text{A.12}) \end{aligned}$$

$$\begin{aligned} \langle x' | \hat{G}_{0,PP}^{\mathcal{P}}(E \pm i0) | x \rangle &= \langle x' | \hat{G}_0(E \pm i0) | x \rangle - \frac{\langle x' | \hat{G}_0(E \pm i0) | \chi_1 \rangle \langle \chi_1 | \hat{G}_0(E \pm i0) | x \rangle}{\langle \chi_1 | \hat{G}_0(E \pm i0) | \chi_1 \rangle} \quad (\text{A.11}) \\ &= \langle x' | \hat{G}_0(E \pm i0) | x \rangle - \frac{2\kappa \hat{e}_2 \hat{e}_2^+}{K_2^*(\kappa + K_2)^2(2\kappa - K_2)} \left( \kappa e^{K_2|x'|} + K_2 e^{-\kappa|x'|} \right) \left( \kappa e^{K_2^*|x|} + K_2^* e^{-\kappa|x|} \right) \quad (4.15) \end{aligned}$$

## 4.2.2 Direct scattering

Even though we do not possess any closed form general solution of direct scattering, we can for our special Hamiltonian apply familiar procedure of solving Lippmann-Schwinger equation used in sections 2.2 and 3.1.

We start with Lippmann-Schwinger equation for  $|(k_n, s, n)^{\mathcal{P}\pm}\rangle$  from (4.2) (in position representation, insertion of the unit operator)<sup>11</sup>

$$\langle x|(k_n, s, n)^{\mathcal{P}\pm}\rangle = \langle x|(k_n, s, n)_0^{\mathcal{P}\pm}\rangle + \int_{\mathbb{R}} dx' \langle x|\widehat{G}_{0,PP}^{\mathcal{P}}(E \pm i0)|x'\rangle \langle x'|\widehat{V}|(k_n, s, n)^{\mathcal{P}\pm}\rangle.$$

As we have already experienced, for the on-shell T matrix  $t_{\text{dir}}(\mathbf{p}' \leftarrow \mathbf{p})$  we would need only terms  $\langle x=0|(k_n, s, n)_0^{\mathcal{P}\pm}\rangle$  and  $\langle x=0|\widehat{G}_{0,PP}^{\mathcal{P}}(E \pm i0)|x'=0\rangle$ . From (4.14) and (4.15) for  $x = x' = 0$  we get

$$\begin{aligned} \langle 0|(k_n, s, n)_0^{\mathcal{P}\pm}\rangle &= \begin{pmatrix} 1 & 0 \\ 0 & \gamma_{\pm} \end{pmatrix} \frac{\hat{e}_n}{\sqrt{2\pi}}, \\ \langle 0|\widehat{G}_{0,PP}^{\mathcal{P}}(E \pm i0)|0\rangle &= \begin{pmatrix} \frac{1}{\pm ik_1} & 0 \\ 0 & \frac{1}{K_2} - \frac{2\kappa(\kappa+K_2^*)}{K_2^*(\kappa+K_2)(2\kappa-K_2)} \end{pmatrix} = \begin{pmatrix} \frac{1}{\pm ik_1} & 0 \\ 0 & \frac{1}{L_2} \end{pmatrix} \end{aligned} \quad (4.16)$$

where

$$L_2 = L_2(E \pm i0) := \begin{cases} \pm ik_2 \rho_{\pm} & , E \geq W \\ -\kappa_2 - 2\kappa & , W > E \geq 0 \end{cases},$$

where for convenience we have defined  $\gamma_{\pm} := \frac{\pm ik_2(\kappa \mp ik_2)}{(2\kappa \mp ik_2)(\kappa \pm ik_2)}$  and  $\rho_{\pm} := \frac{(2\kappa \mp ik_2)(\kappa \pm ik_2)}{4\kappa^2 \mp ik_2(\kappa \pm ik_2)}$ .

Following same steps as before, we get implicit equation

$$\langle x|(k_n, s, n)^{\mathcal{P}\pm}\rangle = \langle x|(k_n, s, n)_0^{\mathcal{P}\pm}\rangle + \langle x|\widehat{G}_{0,PP}^{\mathcal{P}}(E \pm i0)|0\rangle \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \langle 0|(k_n, s, n)^{\mathcal{P}\pm}\rangle,$$

where the undetermined implicit constants  $\langle 0|(k_n, s, n)^{\mathcal{P}\pm}\rangle$  are solved from equation for  $x = 0$

$$\xrightarrow{x=0} \langle 0|(k_n, s, n)^{\mathcal{P}\pm}\rangle = \left[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{\pm ik_1} & 0 \\ 0 & \frac{1}{L_2} \end{pmatrix} \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \right]^{-1} \begin{pmatrix} 1 & 0 \\ 0 & \gamma_{\pm} \end{pmatrix} \frac{\hat{e}_n}{\sqrt{2\pi}}.$$

Using (3.7) we get

$$\langle 0|(k_n, s, n)^{\mathcal{P}\pm}\rangle = -\frac{1}{\sqrt{2\pi}\widetilde{\Delta}_{\pm}} \begin{pmatrix} \pm ik_1(b - L_2) & -cL_2\gamma_{\pm} \\ \mp ic^*k_1 & L_2(a \mp ik_1)\gamma_{\pm} \end{pmatrix} \hat{e}_n, \quad (4.17)$$

where  $\widetilde{\Delta}_{\pm} := (a \mp ik_1)(b - L_2) - |c|^2$ .

For the direct on-shell T matrix  $t_{\text{dir}}(k_n', s', n'; k_n, s, n)$ <sup>12</sup> we can write

$$\begin{aligned} t_{\text{dir}}(k_n', s', n'; k_n, s, n) &= \int_{\mathbb{R}} dx \langle (k_n', s', n')_0^{\mathcal{P}} - |x\rangle \langle x|\widehat{V}|(k_n, s, n)^{\mathcal{P}+}\rangle = \\ &= \langle (k_n', s', n')_0^{\mathcal{P}} - |0\rangle \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} \langle 0|(k_n, s, n)^{\mathcal{P}+}\rangle = \\ &= -\frac{1}{2\pi\widetilde{\Delta}_+} \begin{pmatrix} ik_1(D - aL_2) & ck_1k_2\gamma_+\rho_+ \\ c^*k_1k_2\gamma_+\rho_+ & k_2(iD + bk_1)\gamma_+\rho_+ \end{pmatrix}. \end{aligned}$$

<sup>11</sup>

$$\widehat{G}_0^{\mathcal{P}}(z) \underbrace{\widehat{P}\widehat{V}\widehat{P}}_{\widehat{H}_{PP} - \widehat{T}_{PP}} |\mathbf{p}^{\mathcal{P}\pm}\rangle = \left( \widehat{G}_{0,PP}^{\mathcal{P}}(z) + \widehat{G}_{0,QP}^{\mathcal{P}}(z) \right) \widehat{V} \underbrace{\widehat{P}|\mathbf{p}^{\mathcal{P}\pm}\rangle}_{|\mathbf{p}^{\mathcal{P}\pm}\rangle} = \widehat{G}_{0,PP}^{\mathcal{P}}(z) \widehat{V} |\mathbf{p}^{\mathcal{P}\pm}\rangle$$

<sup>12</sup>

$$t_{\text{dir}}(\mathbf{p}' \leftarrow \mathbf{p}) = \langle \mathbf{p}'_0^{\mathcal{P}} - | \widehat{H}_{PP} - \widehat{T}_{PP} | \mathbf{p}^{\mathcal{P}+} \rangle = \langle \mathbf{p}'_0^{\mathcal{P}} - | \widehat{P}\widehat{V}\widehat{P} | \mathbf{p}^{\mathcal{P}+} \rangle = \langle \mathbf{p}'_0^{\mathcal{P}} - | \widehat{V} | \mathbf{p}^{\mathcal{P}+} \rangle$$

### 4.2.3 Resonant scattering

From theory in the subsection A.14 we know that key matrix elements to calculate the resonant scattering T matrix  $t_{\text{res}}(\mathbf{p}' \leftarrow \mathbf{p})$  are discrete state energy  $H_{11}$  (calculated in Appendix A.2.2, equation (A.14)), discrete-state-continuum coupling  $V_{1,(k_n,s,n)}^\pm$  (calculated in Appendix A.2.2, equation (A.15)) and complex level-shift matrix  $F_{11}(z)$ .

To calculate the last one we start with Lippmann-Schwinger equation for  $\widehat{G}^{\mathcal{P}}(z)$  (1.16) projected to subspace  $\mathcal{P}$  on both sides leading to

$$\widehat{G}_{PP}^{\mathcal{P}}(z) = \widehat{G}_{0,PP}^{\mathcal{P}}(z) + \widehat{G}_{0,PP}^{\mathcal{P}}(z)\widehat{V}\widehat{G}_{PP}^{\mathcal{P}}(z).$$

For spatial matrix elements  $\langle x'|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle$  we get integral equation

$$\langle x'|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle = \langle x'|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|x\rangle + \int_{\mathbb{R}} dy \delta(y) \langle x'|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|y\rangle \Lambda \langle y|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle,$$

where  $\Lambda = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}$ . We already have experience with this type of integral equation (sections 2.2, 3.1 and subsection 4.2.2), so we just skip familiar procedure (implicit equation for  $\langle x'|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle$ , set  $x' = 0$ , express and insert  $\langle 0|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle$ ) and we get

$$\langle x'|\widehat{G}_{PP}^{\mathcal{P}}(z)|x\rangle = \langle x'|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|x\rangle + \langle x'|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|0\rangle \Lambda \left[ \widehat{1} - \langle 0|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|0\rangle \Lambda \right]^{-1} \langle 0|\widehat{G}_{0,PP}^{\mathcal{P}}(z)|x\rangle.$$

Fortunately we will need only spatial matrix element  $\langle 0|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|0\rangle$ , for which the above expression reduces to

$$\begin{aligned} \langle 0|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|0\rangle &= \left[ \widehat{1} - \langle 0|\widehat{G}_{0,PP}^{\mathcal{P}}(E + i0)|0\rangle \Lambda \right]^{-1} \langle 0|\widehat{G}_{0,PP}^{\mathcal{P}}(E + i0)|0\rangle = \\ &= -\frac{1}{\widetilde{\Delta}_+} \begin{pmatrix} b - L_2 & -c \\ -c^* & a - ik_1 \end{pmatrix}. \end{aligned}$$

Inserting to equation (A.17) we get

$$F_{11} = -\frac{\kappa}{\widetilde{\Delta}_+} \left[ (a - ik_1)(\kappa + b)^2 - |c|^2(2\kappa + L_2 + b) \right].$$

We are mostly interested in the case  $W > E \geq 0$ . From equation (4.10) we get

$$t_{\text{res}} = \frac{(V_{1,(k_{n'},s',n')}^-)^* V_{1,(k_n,s,n)}^+}{E - H_{11} - F_{11}(E + i0)} = \frac{k_1^2 \kappa |c|^2}{\pi \Delta_+ \widetilde{\Delta}_+}.$$

We can verify whether the orthogonal, direct and resonant on-shell T matrix add up to total the scattering on-shell T matrix  $t(k_{n'}, s', n'; k_n, s, n)$

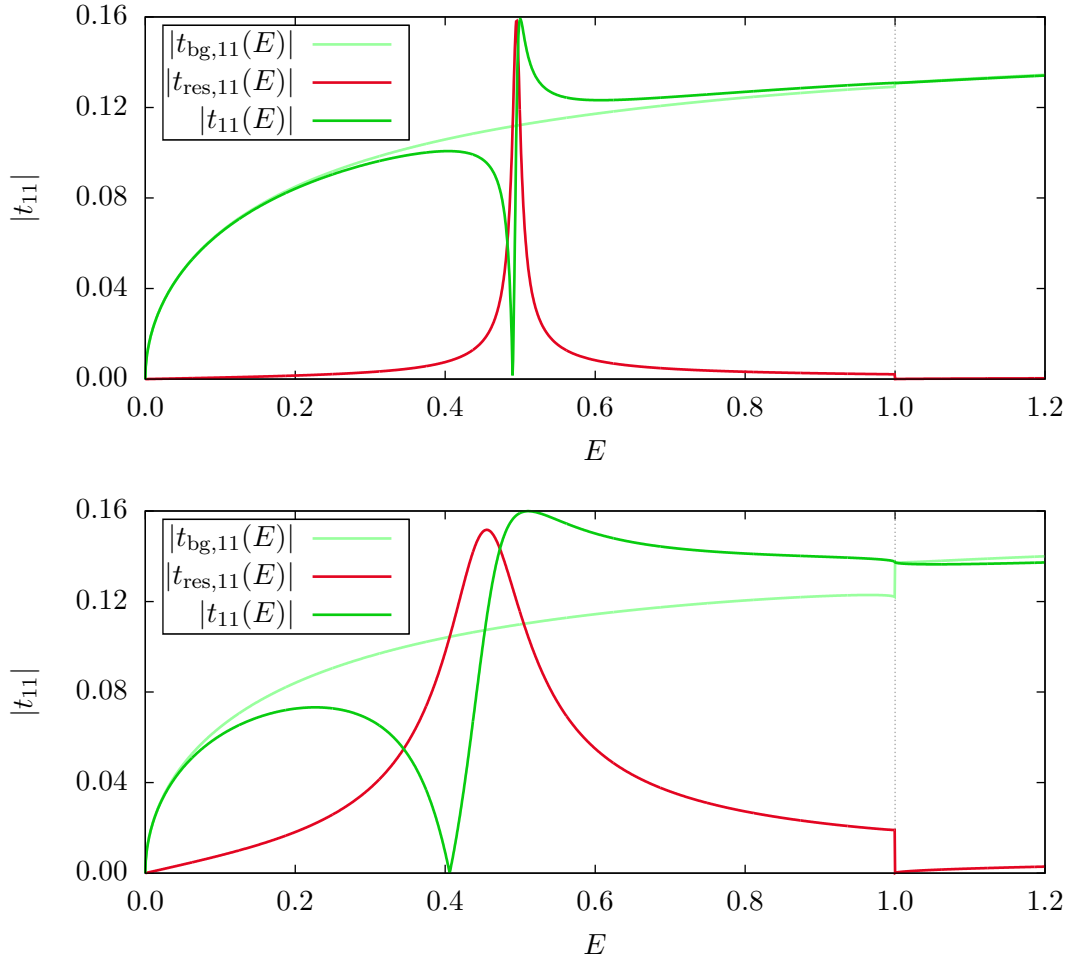
$$\begin{aligned} t &= t_{\text{ortho}} + t_{\text{dir}} + t_{\text{res}} \\ &= 0 - \frac{ik_1 [D + a(\kappa_2 + 2\kappa)]}{2\pi \widetilde{\Delta}_+} + \frac{k_1^2 \kappa |c|^2}{\pi \Delta_+ \widetilde{\Delta}_+} = -\frac{ik_1(D + a\kappa_2)}{2\pi \Delta_+}, \end{aligned}$$

which is in agreement with the total scattering on-shell T matrix  $t(k_{n'}, s', n'; k_n, s, n)$  (deduced from S matrix (3.9))

$$t(k_{n'}, s', n'; k_n, s, n) = -\frac{1}{2\pi \Delta_+} \begin{pmatrix} ik_1(D - aK_2) & ck_1k_2 \\ c^*k_1k_2 & k_2(iD + bk_1) \end{pmatrix}.$$

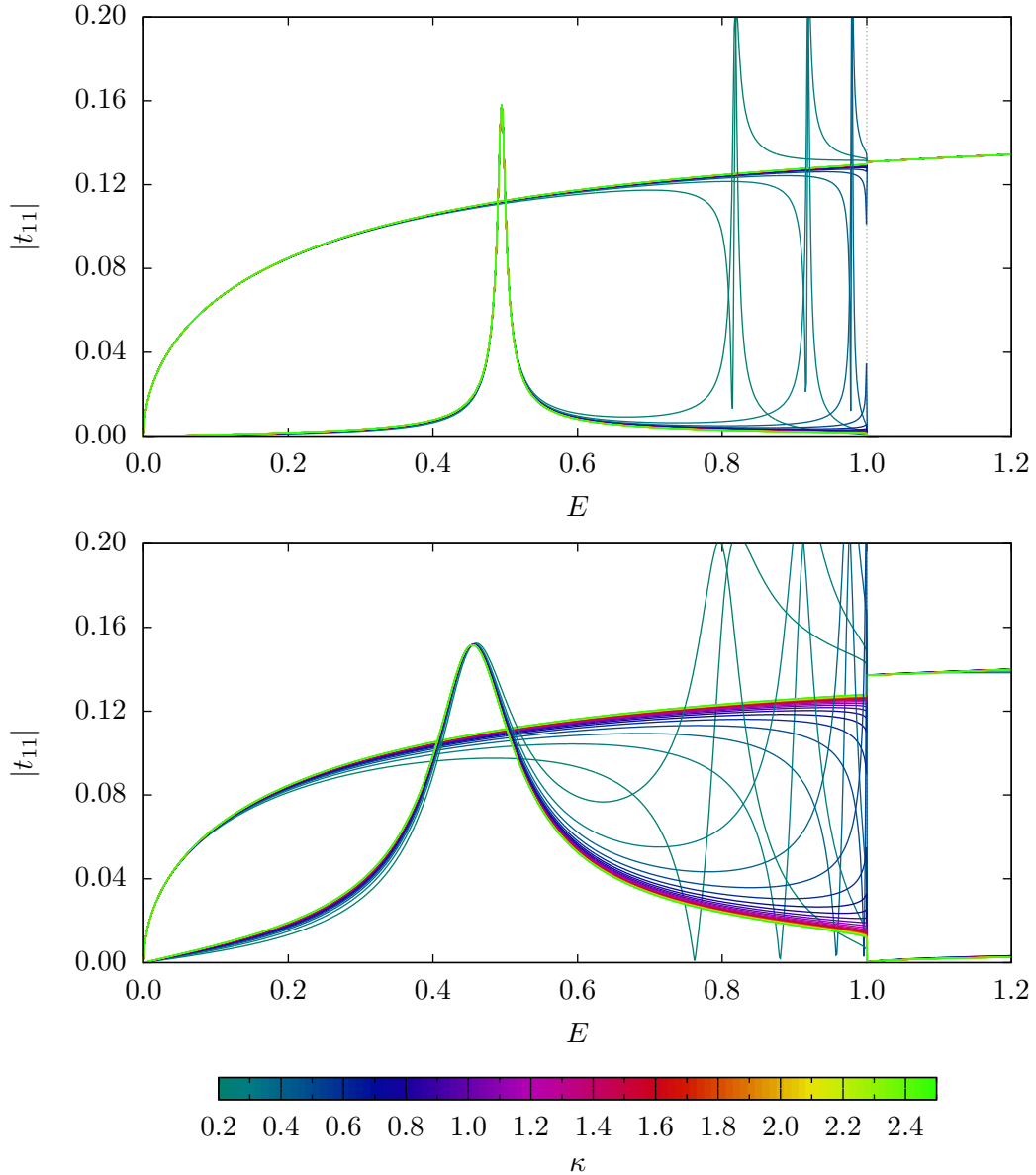
#### 4.2.4 $\kappa$ -dependence

To observe the  $\kappa$ -dependence of the separation first we plot the on-shell T matrix elements for ideal value  $\kappa = -b$  (Figure 4.2). The background on-shell T matrix is the sum of the orthogonal and the direct, but the orthogonal matrix element  $t_{\text{ortho},11}$  is zero. We can see that the separation of the total on-shell T matrix  $t_{11}$  (rapid changes around the resonance energy  $E_r \approx 0.5$ ) to the background scattering term  $t_{\text{bg},11}$  (smooth behaviour) and the resonant term was successful. We can notice that, while the overall on-shell T matrix elements (thus also S matrix elements) are continuous everywhere, the separated terms have one discontinuity at threshold energy  $W$ . This is caused by the discontinuity of the function  $L_2$  defined in (4.16).



**Figure 4.2:** The energy dependence of absolute value of the background ( $t_{\text{bg}}$ ), resonant ( $t_{\text{res}}$ ) and total ( $t$ ) on-shell T matrix element  $t_{11}$  for parameters:  $a = 1$ ,  $b = -1$ ,  $|c| = 0.1$  (the 1st graph);  $a = 1$ ,  $b = -1$ ,  $|c| = 0.3$  (the 2nd graph);  $\kappa = -b = 1$  with marked threshold energy  $W = 1$  (dashed line).

In the Figure 4.3 we can see how the parameter  $\kappa$  affects the separation of the scattering terms. Two effects are observed: in the wide range of values ( $\langle 0.6, 2.5 \rangle$ ) the parameter has minimal if none influence on the separation, which corresponds to fact, that one only needs to estimate the subspace  $\mathcal{Q}$  roughly; for some values ( $\approx \langle 0, 0.5 \rangle$ ) there appears the second, fake resonance peak with corresponding opposite peak in direct scattering. For  $\kappa = 0$  the resonant term is zero and  $t_{11} = t_{\text{bg},11}$ , therefore as we approach this value the separation is worse and worse.



**Figure 4.3:** The dependence of absolute value of the direct and resonant on-shell T matrix element  $t_{11}$  on the parameter  $\kappa$  (from 0.2 to 2.5 with step 0.1; ideally  $\kappa = -b = 1.0$ ) for parameters:  $a = 1, b = -1, |c| = 0.1$  (the 1st graph);  $a = 1, b = -1, |c| = 0.3$  (the 2nd graph), with marked threshold energy  $W = 1$  (dashed line).

#### 4.2.5 Eigenphases

For scattering in full potential we calculated corresponding eigenphases (subsection 3.2.1). We can analogically assign to background and resonant on-shell T matrix corresponding S matrix and consequently eigenphases.<sup>13</sup> But to achieve separation of eigenphases, we cannot directly use relation (1.13). The background scattering is scattering in potential  $\hat{H}_{PP} - \hat{T}$  and corresponding background S matrix  $S_{bg}$  and background eigenphases  $\delta_{bg}$  (the eigenvalue  $e^{2i\delta_{bg}}$ ) can be calculated from background on-shell T mat-

<sup>13</sup>We can also define orthogonal, direct and resonant S matrices and eigenphases, but there is no need to divide background term into two terms.



rix as<sup>14</sup>

$$S_{\text{bg}} = \widehat{1} - 2\pi i t_{\text{bg}}.$$

To preserve unitarity of resonant S matrix and to get simple additive separation of eigenphases, we define altered resonant T matrix  $\tilde{t}_{\text{res}}$

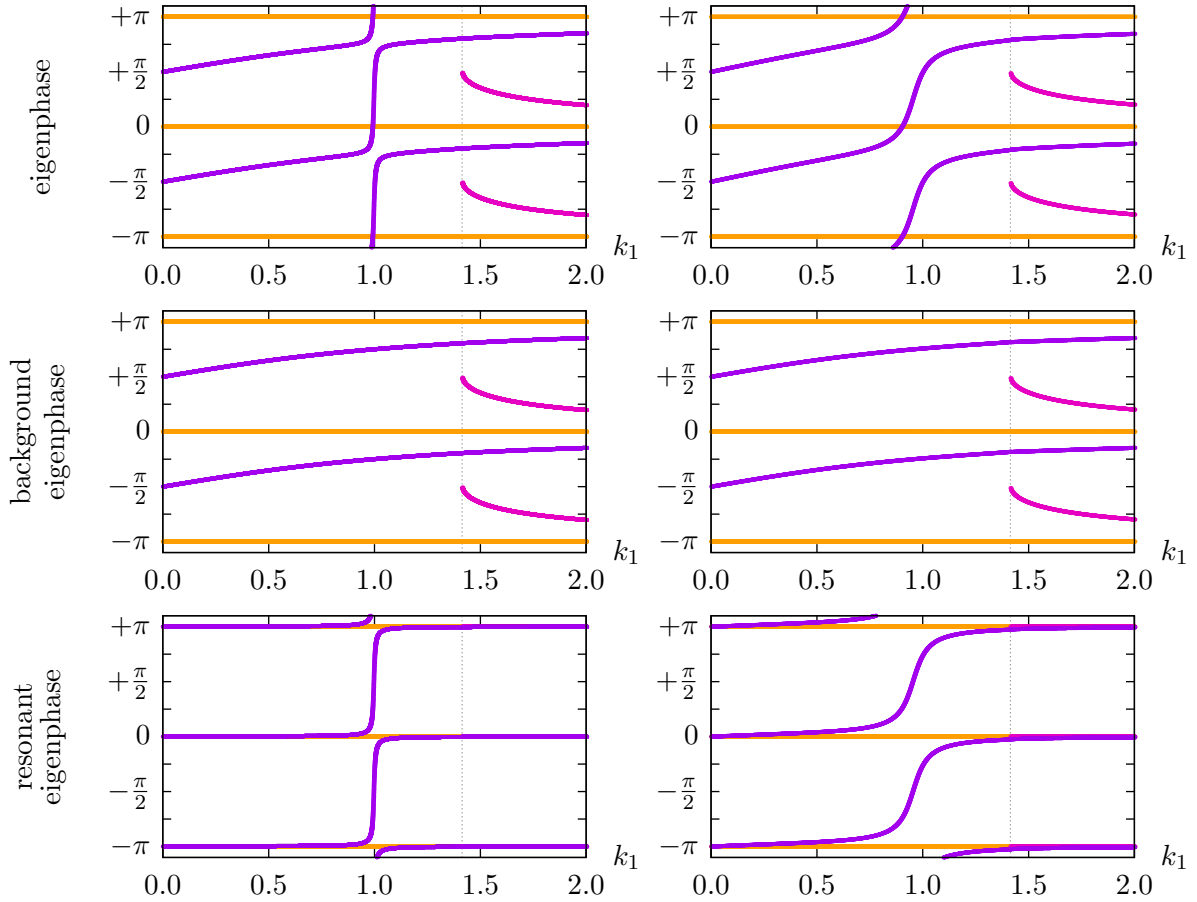
$$\tilde{t}_{\text{res}} = S_{\text{bg}}^{-1} t_{\text{res}},$$

and corresponding resonant S matrix  $S_{\text{res}}$  and resonant eigenphases  $\delta_{\text{res}}$

$$S_{\text{res}} = \widehat{1} - 2\pi i \tilde{t}_{\text{res}}.$$

For S matrices defined like this we can write<sup>15</sup>

$$S = S_{\text{bg}} S_{\text{res}}, \quad \delta = \delta_{\text{bg}} + \delta_{\text{res}}.$$



**Figure 4.4:** Separation of eigenphases  $\delta_1(k_1)$  (violet),  $\delta_{2/4}(k_1)$  (orange) and  $\delta_3(k_1)$  (pink) to background  $\delta_{\text{bg},i}(k_1)$  and resonant  $\delta_{\text{res},i}(k_1)$  eigenphases for parameters:  $a = 1$ ,  $b = -1$ ,  $|c| = 0.1$  (left side);  $a = 1$ ,  $b = -1$ ,  $|c| = 0.3$  (right side);  $\kappa = -b = 1$ .

From given background and resonant on-shell T matrices we calculated corresponding S matrices and using same technique as before (subsections 2.3.1 and 3.2.1) we calculated eigenphases  $\delta_{\text{bg},i}(k_1)$  and  $\delta_{\text{res},i}(k_1)$  for  $i \in \mathbb{N}_1^4$ . The  $k_1$ -dependence of separated and total eigenphases for ideal parameter  $\kappa = -b$  was plotted in Figure 4.4.

We can see, that separation of the background (smooth without rapid changes) eigenphase  $\delta_{\text{bg}}$  and the resonant (step-like) eigenphase  $\delta_{\text{res}}$  for ideal choice of parameter  $\kappa$  was successful.

<sup>14</sup>When calculating we need to be careful to put the normalization term  $1/\sqrt{\kappa_n \kappa_{n'}}$  in the right place.

<sup>15</sup>The second equation applies for one-dimensional matrices.

# Conclusion

In conclusion we would like to summarise achieved results. At first we solved Lippmann-Schwinger equation for one-dimensional two-channel scattering model with delta potential and calculated scattering improper eigenvectors, the S matrix and eigenphases. Out of 5 parameters  $W$ ,  $a$ ,  $b$ ,  $|c|$  and  $\phi$  the model has 3 free parameters  $a$ ,  $b$  and  $|c|$ . We were mostly focused on the most interesting situation with particle incoming in the first channel. The parameter  $a$  determines increasing and decreasing rate for uncoupled ("background") scattering. The parameter  $|c|$  determines strength of coupling and the magnitude of threshold effects (cusps). The parameters  $b$  and  $|c|$  determine the presence (both), position (mainly  $b$ ) and width (mainly  $|c|$ ) of resonances.

The further analysis of the poles of the S matrix in complex  $k$ -plane (two Riemann sheets) shows their mutual relationship with resonances and bound states. Also the change of virtual state to bound states is observed as the change of the limit eigenphase difference  $\delta_1(0) - \delta_1(+\infty)$  by value  $+\pi$ .

Then we applied the projection-operator formalism to explicitly and analytically separate scattering on-shell T matrix to background and resonant part. In the wide range of values of parameter  $\kappa$  (the choice of discrete state) the separation holds with very minimal alternations. Also we managed to separate eigenphases into background and resonant eigenphases.

This model can serve as simple toy model for effects, which occurs in more complicated and complex calculations (e.g. electron – molecule collisions).

# A. Appendices

## A.1 The matrix elements of the free Green's operator $\widehat{G}_0(z)$

For our purposes we need to find the matrix elements of the free Green's operator  $\widehat{G}_0(z)$  for one-dimensional Hamiltonian  $\widehat{H}_0$ .<sup>1</sup>

We recall the definition (1.14) of the free Green's operator  $\widehat{G}_0(z)$

$$\widehat{G}_0(z) := \left( z - \widehat{H}_0 \right)^{-1},$$

and using property (1.2) we get the full set of eigenvectors  $|p\rangle$

$$\widehat{G}_0(z)|p\rangle = \frac{1}{z - E_p}|p\rangle. \quad (\text{A.1})$$

For the momentum matrix elements of the free Green's operator  $\langle p'|\widehat{G}_0(z)|p\rangle$  it is straight-forward

$$\langle p'|\widehat{G}_0(z)|p\rangle = \frac{1}{z - E_p}\langle p'|p\rangle = \frac{1}{z - E_p}\delta(p' - p).$$

For the spatial matrix elements of the free Green's operator  $\langle x'|\widehat{G}_0(z)|x\rangle$  using the spectral decomposition of the unit operator  $\widehat{1}$  we obtain (compare the middle term to (1.15))

$$\begin{aligned} \langle x'|\widehat{G}_0(z)|x\rangle &= \langle x'|\widehat{G}_0(z)\widehat{1}|x\rangle = \int_{-\infty}^{+\infty} dp \langle x'|\widehat{G}_0(z)|p\rangle \langle p|x\rangle \stackrel{(\text{A.1})}{=} \\ &\stackrel{(\text{A.1})}{=} \int_{-\infty}^{+\infty} dp \frac{\langle x'|p\rangle \langle p|x\rangle}{z - E_p} \stackrel{(1.1)}{=} \frac{1}{2\pi} \int_{-\infty}^{+\infty} dp \frac{e^{ip(x'-x)}}{z - E_p} \stackrel{(1.11)}{=} \frac{1}{\pi} \int_{-\infty}^{+\infty} dp \frac{e^{ip(x'-x)}}{2z - p^2}. \end{aligned}$$

To evaluate the integral we need to use basic tools of complex analysis: *Cauchy's residue theorem*<sup>2</sup> and *Jordan's lemma*<sup>4</sup>.

<sup>1</sup>Same procedure can be used for multi-dimensional case, the trick is to use the spherical coordinate system with  $\hat{z} = \hat{p}$ .

<sup>2</sup>*Cauchy's residue theorem.* Let

- $\Omega \subset \mathbb{C}$  be simply connected<sup>3</sup>open subset of the complex plane,
- $\{p_j\}_{j=1}^N \in \Omega$  be finite points of subset  $\Omega$ ,
- $f(p)$  be analytic function on  $\Omega \setminus \{p_j\}_{j=1}^N$ ,
- $\gamma$  be closed path in  $\Omega \setminus \{p_j\}_{j=1}^N$ ,

then

$$\oint_{\gamma} dp f(p) = 2\pi i \sum_{j=1}^N \text{ind}(\gamma, p_j) \text{res}(f, p_j), \quad (\text{A.2})$$

where  $\text{ind}(\gamma, p_j)$  is *winding number* (the total number of times that path  $\gamma$  travels counterclockwise around the point  $p_j$ ) and  $\text{res}(f, p_j)$  is *residue* (the coefficient  $c_{-1}$  in the Laurent series of function  $f(p)$ )

at the point  $p_j$ ,  $f(p) = \sum_{n=-\infty}^{+\infty} c_n (p - p_j)^n$ .

<sup>3</sup>1. Every two points of the set are connected with continuous path in this set.

2. Every path between two fixed points can be continuously transformed into any other path.

<sup>4</sup>*Jordan's lemma.* Let

- $C_R := \{Re^{i\phi} | \phi \in (0, \pi)\}$  be semicircular contour of radius  $R > 0$  lying in the upper half-plane,

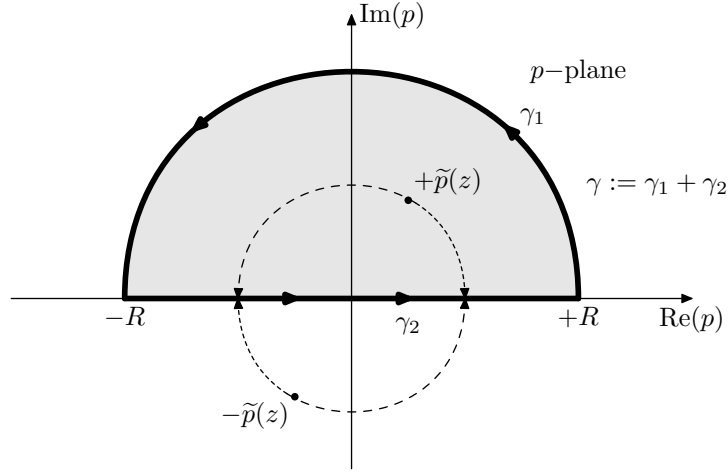
### A.1.1 Non-negative energy ( $E \geq 0$ )

First, we are interested in the matrix elements of the limit operator  $\widehat{G}_0(E_p \pm i0) := \lim_{\varepsilon \rightarrow +0} \widehat{G}_0(E_p \pm i\varepsilon)$  (in other words for non-negative energy). The function  $f(p) := \frac{e^{ip(x'-x)}}{2z-p^2}$  as function of the complex variable  $p$  has 2 simple poles (for  $|z| > 0$ , which is always the case<sup>5</sup>) at points  $p_1 = +\tilde{p}(z)$  and  $p_2 = -\tilde{p}(z)$ , where  $\tilde{p}(z) := \sqrt{2z}$ . It can be rewritten into the form

$$f(p) = \frac{e^{ip(x'-x)}}{2z-p^2} = \frac{e^{ip(x'-x)}}{2\tilde{p}(z)} \left( \frac{1}{p+\tilde{p}(z)} - \frac{1}{p-\tilde{p}(z)} \right). \quad (\text{A.4})$$

We distinguish three cases:

1.  $(x' - x) > 0$ . Let  $R > |\tilde{p}(z)| > 0$  be radius and choose closed contour  $\gamma$  as seen in Figure A.1. The contour  $\gamma := \gamma_1 + \gamma_2$  consists of two path:  $\gamma_1$  – semicircle of radius  $R$  from the point  $+R$  to  $-R$ ,  $\gamma_2$  – straight line along the real axis from point  $-R$  to  $+R$ .



**Figure A.1:** The contour of integration  $\gamma$  in complex  $p$ -plane.

Now we will look at Cauchy integral of function  $f(p)$  over the contour  $\gamma$ :

$$\int_{C_R} dp f(p) + \int_{-R}^{+R} dp f(p) \stackrel{\gamma := \gamma_1 + \gamma_2}{=} \oint_{\gamma} dp f(p) \stackrel{(\text{A.2})}{=} 2\pi i \sum_{j=1}^2 \text{ind}(\gamma, p_j) \text{res}(f, p_j). \quad (\text{A.5})$$

From Figure A.1 we know  $\text{ind}(\gamma, p_1) = 1$  and  $\text{ind}(\gamma, p_2) = 0$  and from the expression (A.4) we can see values of the residues  $\text{res}(f, p_1) = -\frac{e^{ip_1(x'-x)}}{2\tilde{p}(z)}$  and  $\text{res}(f, p_2) = \frac{e^{ip_2(x'-x)}}{2\tilde{p}(z)}$ .

$$\int_{C_R} dp f(p) + \int_{-R}^{+R} dp f(p) = -\frac{\pi i}{\tilde{p}(z)} e^{i\tilde{p}(z)(x'-x)}$$

---

•  $f(p) = e^{iap} g(p)$  be continuous complex function with a positive parameter  $a > 0$  defined at  $C_R$ , then

$$\left| \int_{C_R} dp f(p) \right| \leq \frac{\pi}{a} \max_{\phi \in (0, \pi)} |g(Re^{i\phi})|. \quad (\text{A.3})$$

<sup>5</sup>

$$|z| = (E_p^2 + \epsilon^2)^{1/2} \geq \epsilon > 0$$

Now we are interested in limit  $R \rightarrow +\infty$ .

$$\lim_{R \rightarrow +\infty} \int_{C_R} dp f(p) + \int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi i}{\tilde{p}(z)} e^{i\tilde{p}(z)(x'-x)}$$

Using Jordan's lemma (A.3) for  $g(p) = \frac{1}{2z-p^2}$  and  $a = (x' - x)$  we get

$$\begin{aligned} \lim_{R \rightarrow +\infty} \left| \int_{C_R} dp f(p) \right| &\stackrel{(A.3)}{\leq} \lim_{R \rightarrow +\infty} \frac{\pi}{(x' - x)} \max_{\phi \in (0, \pi)} \left| \frac{1}{2z - R^2 e^{2i\phi}} \right| = \\ &= \lim_{R \rightarrow +\infty} \frac{\pi}{(x' - x)} \frac{1}{R^2 - 2|z|} = 0, \end{aligned}$$

what directly implies

$$\lim_{R \rightarrow +\infty} \int_{C_R} dp f(p) = 0 \quad (\text{A.6})$$

and we obtained required result

$$\int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi i}{\tilde{p}(z)} e^{i\tilde{p}(z)(x'-x)}$$

2.  $(x' - x) = 0$ . We follow exactly same procedure as in the previous case and end up with same result for  $(x' - x) = 0$ . Only argumentation for zero integral

$\lim_{R \rightarrow +\infty} \int_{C_R} dp f(p)$  will be different.

$$\begin{aligned} \lim_{R \rightarrow +\infty} \left| \int_{C_R} dp f(p) \right| &= \left\| \frac{p=Re^{i\phi}}{dp=Re^{i\phi}d\phi} \right\| = \lim_{R \rightarrow +\infty} \left| \int_0^\pi d\phi f(Re^{i\phi}) Rie^{i\phi} \right| \leq \\ &\leq \lim_{R \rightarrow +\infty} \int_0^\pi d\phi \left| f(Re^{i\phi}) Rie^{i\phi} \right| \leq \lim_{R \rightarrow +\infty} \int_0^\pi d\phi \max_{\phi \in (0, \pi)} \left| f(Re^{i\phi}) \right| R = \\ &= \lim_{R \rightarrow +\infty} \int_0^\pi d\phi \frac{R}{R^2 - 2|z|} = \lim_{R \rightarrow +\infty} \frac{\pi R}{R^2 - 2|z|} = 0 \end{aligned}$$

3.  $(x' - x) < 0$ . Firstly we substitute  $p' = -p$

$$\int_{-\infty}^{+\infty} dp f(p) = \left\| \frac{p'=-p}{dp'=-dp} \right\| = - \int_{+\infty}^{-\infty} dp' \frac{e^{-ip'(x'-x)}}{2z - p'^2} = \int_{-\infty}^{+\infty} dp' \frac{e^{ip'[-(x'-x)]}}{2z - p'^2},$$

which leads to the same integral as in the first case for  $[-(x' - x)] > 0$ , therefore the result is

$$\int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi i}{\tilde{p}(z)} e^{i\tilde{p}(z)[-(x'-x)]}.$$

Result for all three cases can put into single formula

$$\int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi i}{\tilde{p}(z)} e^{i\tilde{p}(z)|x'-x|},$$

which gives us

$$\langle x' | \hat{G}_0(z) | x \rangle = -\frac{i}{\tilde{p}(z)} e^{i\tilde{p}(z)|x'-x|}.$$

At last, we need to proceed limit  $\lim_{\epsilon \rightarrow +0} E_p \pm i\epsilon := E_p \pm i0$ , what can be done using Figure A.1. For  $+\epsilon > 0$  the value  $+\tilde{p}(z)$  approaches value  $+\tilde{p}(z) \rightarrow +p$  (densely dashed arrow), for  $-\epsilon < 0$  the value  $+\tilde{p}(z)$  approaches value  $+\tilde{p}(z) \rightarrow -p$  (loosely dashed arrow).

The final result is

$$\langle x' | \hat{G}_0(E_p \pm i0) | x \rangle = \pm \frac{1}{ip} e^{\pm ip|x'-x|}. \quad (\text{A.7})$$

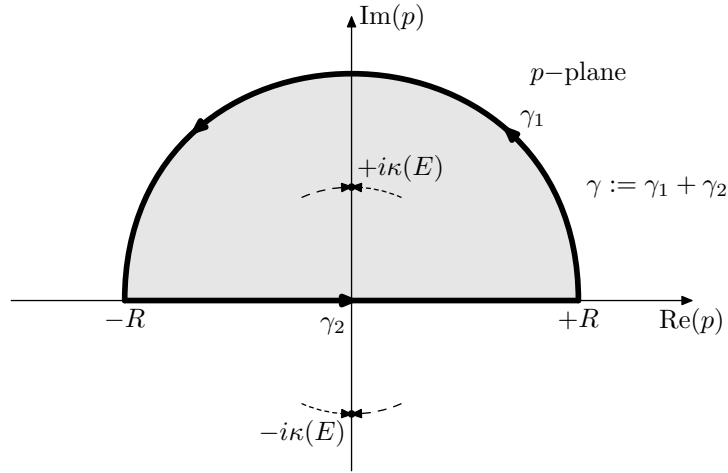
### A.1.2 Negative energy ( $E < 0$ )

Second, we will evaluate the spatial matrix elements of the operator  $\widehat{G}_0(E)$  for negative energy  $E$ .<sup>6</sup> For negative energy we define  $\kappa(E) := \sqrt{-2E}$ . As before, the function  $f(p)$  has 2 simple poles at points  $p_1 = +i\kappa(E)$  and  $p_2 = -i\kappa(E)$ , thus we can  $f(p)$  rewrite as

$$f(p) = \frac{e^{ip(x'-x)}}{2E - p^2} = \frac{-ie^{ip(x'-x)}}{2\kappa(E)} \left( \frac{1}{p + i\kappa(E)} - \frac{1}{p - i\kappa(E)} \right). \quad (\text{A.8})$$

In the same fashion as before, we distinguish three cases:

1.  $(x' - x) > 0$ . Let  $R > \kappa(E) > 0$  be radius and choose the same closed contour  $\gamma$  as previously (Figure A.2).



**Figure A.2:** The contour of integration  $\gamma$  in complex  $p$ -plane.

Again we will express the Cauchy integral of function  $f(p)$  over the contour  $\gamma$  (A.5). From Figure A.2 we get  $\text{ind}(\gamma, p_1) = 1$  and  $\text{ind}(\gamma, p_2) = 0$  and from the expression (A.8) we deduce values of the residues  $\text{res}(f, p_1) = \frac{ie^{-\kappa(E)(x'-x)}}{2\kappa(E)}$  and  $\text{res}(f, p_2) = \frac{-ie^{+\kappa(E)(x'-x)}}{2\kappa(E)}$ . Proceeding the limit  $R \rightarrow +\infty$  and using the result of Jordan's lemma (A.6) we get

$$\int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi}{\kappa(E)} e^{-\kappa(E)(x'-x)}.$$

2.  $(x' - x) = 0$ . Same procedure as before leading to the same result for  $(x' - x) = 0$ . Argumentation for zero semicircle integral is same as for non-negative energy.
3.  $(x' - x) < 0$ . Using same substitution as for non-negative energy we obtain the same result for  $[-(x' - x)] > 0$ .

Putting all cases into single formula gives us

$$\int_{-\infty}^{+\infty} dp f(p) = -\frac{\pi}{\kappa(E)} e^{-\kappa(E)|x'-x|} \implies \langle x' | \widehat{G}_0(E) | x \rangle = -\frac{1}{\kappa(E)} e^{-\kappa(E)|x'-x|}. \quad (\text{A.9})$$

<sup>6</sup>According to analyticity of the free Green's operator  $\widehat{G}_0(z)$  (Figure 1.3) for non-negative energy we had to use limit, but for negative energy the limit is equal to defined operator for real  $z$  as we will see.

As we can see in Figure A.2 the whole process with limits  $\lim_{\varepsilon \rightarrow +0} E \pm i\varepsilon$  would lead to the same result. Either for  $+\varepsilon > 0$  (densely dashed arrows) or for  $-\varepsilon < 0$  (loosely dashed arrow)

$$\langle x' | \widehat{G}_0(E \pm i0) | x \rangle = \langle x' | \widehat{G}_0(E) | x \rangle.$$

## A.2 Computation of matrix elements in projection-operator formalism

In this appendix we will outline ways, how the matrix elements in projection-operator formalism have been evaluated. In general, the technique involves: insertion of unit operator ( $\widehat{1} = \int_{\mathbb{R}} dx |x\rangle \langle x|$ ), insertion of already known matrix elements and evaluation of a simple integral (integration with delta function  $\delta(x)$  or exponential<sup>7</sup>  $e^{-\alpha|x-x_0|}$ ).

### A.2.1 Orthogonal scattering

$$\begin{aligned} \langle \chi_1 | k_n, s, n \rangle &= \int_{\mathbb{R}} dx \langle \chi_1 | x \rangle \langle x | k_n, s, n \rangle \stackrel{(4.13)}{=} \stackrel{(3.2)}{=} \\ &= \hat{e}_2^+ \hat{e}_n \sqrt{\frac{\kappa}{2\pi}} \int_{\mathbb{R}} dx e^{-\kappa|x| + isk_n x} = \delta_{2n} \sqrt{\frac{\kappa}{2\pi}} \frac{2\kappa}{\kappa^2 + k_2^2} \end{aligned} \quad (\text{A.10})$$

$$\begin{aligned} \langle x | \widehat{G}_0(E \pm i0) | \chi_1 \rangle &= \int_{\mathbb{R}} dx' \langle x | \widehat{G}_0(E \pm i0) | x' \rangle \langle x' | \chi_1 \rangle \stackrel{(3.4)}{=} \stackrel{(4.13)}{=} \\ &= \frac{\sqrt{\kappa} \hat{e}_2}{K_2} \int_{\mathbb{R}} dx' e^{K_2|x-x'| - \kappa|x'|} = \frac{2\sqrt{\kappa} \hat{e}_2}{K_2(\kappa^2 - K_2^2)} \left( \kappa e^{K_2|x|} + K_2 e^{-\kappa|x|} \right) \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned} \langle \chi_1 | \widehat{G}_0(E \pm i0) | \chi_1 \rangle &= \int_{\mathbb{R}} dx \langle \chi_1 | x \rangle \langle x | \widehat{G}_0(E \pm i0) | \chi_1 \rangle \stackrel{(A.11)}{=} \stackrel{(4.13)}{=} \\ &= \frac{2\kappa \hat{e}_2^+ \hat{e}_2}{K_2(\kappa^2 - K_2^2)} \int_{\mathbb{R}} dx \left( \kappa e^{(K_2 - \kappa)|x|} + K_2 e^{-2\kappa|x|} \right) = \frac{2(2\kappa - K_2)}{K_2(\kappa - K_2)^2} \end{aligned} \quad (\text{A.12})$$

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<sup>7</sup>The integral with exponential  $e^{-\alpha|x-x_0|}$  is split into two integrals over two intervals  $(-\infty, x_0)$  and  $(x_0, +\infty)$ , which are simple.

## A.2.2 Resonant scattering

$$\begin{aligned}
\langle x|\widehat{H}|\chi_1\rangle &\stackrel{(4.13)}{=} \stackrel{(3.1)}{=} \left(-\frac{1}{2}\frac{d^2}{dx^2} + W + b\delta(x)\right) \sqrt{\kappa}e^{-\kappa|x|} = \left(-\frac{1}{2}\kappa^2 + \kappa\delta(x) + W + b\delta(x)\right) \sqrt{\kappa}e^{-\kappa|x|} = \\
&= \sqrt{\kappa} \begin{pmatrix} c \\ b + \kappa \end{pmatrix} \delta(x) + \left(-\frac{1}{2}\kappa^2 + W\right) \langle x|\chi_1\rangle \tag{A.13}
\end{aligned}$$

$$\begin{aligned}
H_{11} &= \langle \chi_1|\widehat{H}|\chi_1\rangle = \int_{\mathbb{R}} dx \langle \chi_1|x\rangle \langle x|\widehat{H}|\chi_1\rangle \stackrel{(4.13)}{=} \stackrel{(A.13)}{=} \\
&= \int_{\mathbb{R}} dx \left[ (b + \kappa)\delta(x) + \left(-\frac{1}{2}\kappa^2 + W\right) \right] \kappa e^{-2\kappa|x|} = W + \frac{1}{2}\kappa^2 + b\kappa \tag{A.14}
\end{aligned}$$

$$\begin{aligned}
V_{1,(k_n,s,n)}^\pm &= \langle \chi_1|\widehat{H}|(k_n, s, n)^{\mathcal{P}\pm}\rangle = \int_{\mathbb{R}} dx \langle \chi_1|\widehat{H}|x\rangle \langle x|(k_n, s, n)^{\mathcal{P}\pm}\rangle \stackrel{(A.13)}{=} \\
&= \int_{\mathbb{R}} dx \delta(x) \sqrt{\kappa} \begin{pmatrix} c^* & b + \kappa \end{pmatrix} \langle x|(k_n, s, n)^{\mathcal{P}\pm}\rangle + \left(-\frac{1}{2}\kappa^2 + W\right) \langle \chi_1|(k_n, s, n)^{\mathcal{P}\pm}\rangle \stackrel{(4.17)}{=} \\
&= -\sqrt{\frac{\kappa}{2\pi}} \frac{1}{\widetilde{\Delta}_\pm} (\mp ik_1 c^* (L_2 + \kappa) - L_2 \gamma_\pm [(a \mp ik_1)(b + \kappa) - |c|^2]) \hat{e}_n \tag{A.15}
\end{aligned}$$

$$\begin{aligned}
\langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)\widehat{H}|\chi_1\rangle &= \int_{\mathbb{R}} dy \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|y\rangle \langle y|\widehat{H}|\chi_1\rangle \stackrel{(A.13)}{=} \\
&= \int_{\mathbb{R}} dy \delta(y) \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|y\rangle \sqrt{\kappa} \begin{pmatrix} c \\ b + \kappa \end{pmatrix} + \\
&+ \left(-\frac{1}{2}\kappa^2 + W\right) \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|\chi_1\rangle \stackrel{(4.17)}{=} \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|0\rangle \sqrt{\kappa} \begin{pmatrix} c \\ b + \kappa \end{pmatrix} \tag{A.16}
\end{aligned}$$

$$\begin{aligned}
F_{11} &= \langle \chi_1|\widehat{H}\widehat{G}_{PP}^{\mathcal{P}}(E + i0)\widehat{H}|\chi_1\rangle = \int_{\mathbb{R}} dx \langle \chi_1|\widehat{H}|x\rangle \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)\widehat{H}|\chi_1\rangle \stackrel{(A.16)}{=} \\
&= \int_{\mathbb{R}} dx \delta(x) \sqrt{\kappa} \begin{pmatrix} c^* & b + \kappa \end{pmatrix} \langle x|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)\widehat{H}|\chi_1\rangle + \\
&+ \left(-\frac{1}{2}\kappa^2 + W\right) \langle \chi_1|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)\widehat{H}|\chi_1\rangle \stackrel{(A.16)}{=} \\
&= \kappa \begin{pmatrix} c^* & b + \kappa \end{pmatrix} \langle 0|\widehat{G}_{PP}^{\mathcal{P}}(E + i0)|0\rangle \begin{pmatrix} c \\ b + \kappa \end{pmatrix} \tag{A.17}
\end{aligned}$$



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