General inner products for energy eigenstates

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Abstract. The features of the inner products between all the types of real and complex-energy solutions of the Schrödinger equation for 1-dimensional cut-off quantum potentials are worked out using a Gaussian regularization. A general Master Solution is introduced which describes any of the above solutions as particular cases. From it, a Master Inner Product is obtained which yields all the particular products. We show that the Outgoing and the Incoming Boundary Conditions fully determine the location of the momenta respectively in the lower and upper half complex plane even for purely imaginary momenta (anti-bound and bound solutions).

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1. Introduction

The (time-independent) Schrödinger Equation (SE) has a variety of solutions according to the Boundary Conditions we impose on them. Besides the physical bound eigenstates ($\tilde{\phi}_i$ with discrete negative real energy spectrum and positive purely imaginary momenta) we have marginally physical ones (continuum of positive real energy scattering solutions $\psi_E$), complex-energy solutions (resonances $u_n$), the also unphysical anti-bound states ($\phi_i$ with negative purely imaginary momenta), and, finally, a complex-energy continuum of "background" states ($u_E$). Out of these states, only the bound states have a finite norm (that is, $\tilde{\phi}_i \in L^2$, the Hilbert space).

The properties and uses of the real-energy bound and scattering (Dirac) states are a standard textbook topic on foundations of quantum mechanics. Also the resonances (known as Gamow states [1]) have deserved extensive attention in the literature as descriptive of decaying states. However they feature a spatially divergent asymptotic behaviour, which leads to infinite norms and seemingly divergent inner products. This problem has historically hampered the study of these solutions and spurred several attempts to circumvent it by trying different regularization prescriptions. Examples of this are analytical continuations of the inner products in the complex momentum plane, the External Complex Scaling of the space coordinate, and the introduction of convergence factors in the space integrals. The interested reader may find some bibliographical cues on these proposals in [2] [3] [4]. In [4] the Gaussian regularization has been used to achieve new results on the computation of the inner products involving resonances.

In this paper we complete our previous results, obtained for a general 1-dimensional potential with finite support, by considering the full set of solutions of the SE including the anti-bound and the "background" states.

In Section 2, we first characterize the solutions according to the Boundary Conditions (BCs) they obey, having the Outgoing (OBCs) and Incoming (IBCs) Boundary Conditions a chief role. We will show that also the bound and anti-bound solutions fit in the ensuing classification. We then introduce a general form of the solution to the SE as a Master Solution (MS) from which all the solutions above stem as particular cases.

In Section 3 we exploit this Master Solution to obtain a compact Master Inner Product (MIP) from which the table of the particular inner products between all the solutions can be worked out. This general framework lets us to see how the different kinds of orthogonality, namely Kronecker-$\delta$, Dirac-$\delta$, or other, stem from a common expression.

In Section 4 the Conclusions are drawn. The details of some calculations and the basic integral formulas are deferred to Appendices.
2. Solutions and Boundary Conditions

We consider the 1-D time-independent Schrödinger equation

\[ \left( \frac{\partial^2}{\partial x^2} + p^2 - 2mV(x) \right) \psi(x, p) = 0 \]  

(1)

where we have used units such that \( \hbar = 1 \), and a cut-off potential \( V(x) \) describing a general barrier with support in the compact interval \([0, L]\). We also assume that the potential features local negative minima (wells) such that bound states occur.

Besides the better known scattering in and out solutions for continuous real energy \( E = p^2/2m > 0 \) and the bound and anti-bound states (discrete real \( E_i < 0 \)), one has resonant solutions satisfying the Siegert Boundary Conditions [5], and the more general continuous complex-energy ”background” solutions. Here we briefly highlight some of their features and introduce our systematics together with some notation. We also stress that outside \([0, L]\) the solutions already adopt their Asymptotic Form (AF) for \( x \to \pm \infty \), the use of which may be a convenient alternative to their BCs at \( x = 0, L \) (or at \( x = \pm \infty \)). The BCs maybe algebraic or differential and the general setup is that imposing one BC leaves the functional degree of freedom corresponding to a continuum (energy or momentum) spectrum, as is the case of the scattering and background solutions, whereas two BCs over-determine the problem yielding a discrete spectrum, whether of real energies (bound and anti-bound solutions) or complex energies (resonances). Graphical representations of the location of the momenta of the different solutions in the complex-momentum plane can be found in [4].

2.1. Bound and anti-bound states

The bound states \( \tilde{\phi}_i \) are the only solutions \( \in L^2 \) and they are characterized by the AF

\[ \tilde{\phi}_i(x) = \begin{cases} R_i e^{\tilde{q}_i x} & , \ x \leq 0 \\ T_i e^{-\tilde{q}_i x} & , \ x \geq L \end{cases} \]

where \( \tilde{q}_i > 0 \). This is equivalent to imposing the BCs

\[ \partial_x \tilde{\phi}|_{x=0} = \tilde{q} \tilde{\phi}(0), \quad \partial_x \tilde{\phi}|_{x=L} = -\tilde{q} \tilde{\phi}(L) \ (\tilde{q} > 0), \]

(3)

which imply the weaker BCs \( \tilde{\phi}_i(\pm \infty) = 0 \). The anti-bound solutions instead correspond to the mirror values \( q_i = -\tilde{q}_i < 0 \) in (2) and (3), then becoming \( \notin L^2 \) (thus dubbed unphysical), and have the same negative energies \( E_i = -q_i^2/2m \).

The AF of both types of solutions maybe viewed as plane waves (say \( e^{ipx} \) in the right side of the barrier) with purely imaginary ”momenta” \( p \), which may lie in the positive imaginary axis \( \mathcal{I}_+ \) (bound states) or in the negative one \( \mathcal{I}_- \) (anti-bound solutions). This interpretation makes these states akin to the resonances. The tilde notation we have adopted for the bound solutions reflects their relationship with the Incoming resonances below.
2.2. Resonances

They are characterized by the Siegert homogeneous *Outgoing* BCs (OBCs)

\[ \partial_x u_{x=0} = -i p u(0) , \quad \partial_x u_{x=L} = i p u(L) , \]

from where (3) is recovered as the particular case of purely imaginary momenta \( p = iq \).

Solutions \( u_n(x) \), called proper resonances, exist for a denumerable set of isolated complex values \( p_n \) of \( p \) (with corresponding complex energies \( Z_n = p_n^2/(2m) \) lying inside the octants close to the real axis (i.e. \( |\text{Re} p_n| > |\text{Im} p_n| \) in the lower half complex plane \( \mathbb{C}_- \) (i.e. \( \text{Im} p_n < 0 \)), and occupy symmetrical positions with respect to the imaginary axis. It is customary to label them as \( p_n \) \((n = 1, 2, ...)\) when \( \text{Re} p_n > 0 \) and as \( p_{-n} \equiv -p_n^* \) their symmetric ones, some times called anti-resonances. The real parts \( \text{Re} p_n \) tend to be spaced regularly for increasing \(|n|\), while \( |\text{Im} p_n| \) grows slowly [6].

BCs with reversed sign of \( p \) in (4) (call them IBCs) correspond to *Incoming* solutions \( \tilde{u}_n(x) \). For real potentials \( V(x) \) one has that \( \tilde{u}_n(x) = u_n^*(x) \), and the momenta \( \tilde{p}_n = p_n^* \) lie in the upper half complex plane \( \mathbb{C}_+ \). We denote with \( |\tilde{z}_n\rangle \) these states. As stressed above, the bound states maybe viewed as Incoming resonances with zero real part momenta, whereas the anti-bound solutions would be particular cases of the Outgoing resonances.

The OBCs are equivalent to imposing the asymptotic form

\[ u_n(x) = \begin{cases} R_n e^{-ip_n x} & , \quad x \leq 0 \\ T_n e^{ip_n x} & , \quad x \geq L \end{cases} \]

(5)

where the amplitudes \( R_n \) and \( T_n \) differ by a phase and are defined up to a global arbitrary normalization factor. An immediate consequence is that the norm is even more divergent than for the Dirac states, causing both kinds of states not to belong to \( L^2 \). Moreover, inner products involving resonant (as well as any other non-normalizable) states, maybe expected to be generally divergent as well, so that their actual calculation requires a regularization.

2.3. Scattering solutions

The continuum spectrum of the scattering states maybe characterized by just one BC, which can be taken at \( x = 0 \) or \( x = L \) and chosen to be of the Outgoing or of the Incoming type, with an obvious corresponding AF. Let us call SBCs any of these choices. For instance, a right-moving *in* state obeys only the second OBC in (4) with \( p > 0 \). This is equivalent to imposing the following form

\[ \psi_r^+(x) = N(p) \begin{cases} e^{ipx} + R(p) e^{-ipx} & , \quad x \leq 0 \\ N^{-1} \psi_r^+(x) & , \quad 0 < x < L \\ T(p) e^{ipx} & , \quad x \geq L \end{cases} \]

(6)

where the form of the solution in \([0, L]\) depends on \( V(x) \), and we adopt the \( \delta \)-energy wave function normalization \( N(p) = m^{1/2} \sqrt{2}\pi p \). We stress here that the customary *in-out* notation for the scattering states is misleading as referring to the BCs they obey,
as long as OBCs correspond to in states, like (6), whereas IBCs yield the out states \( \psi_{\text{out}}(x) \).

2.4. Complex extension, background states, and Master Solution

The continuation to the complex plane of the scattering solutions \( \psi_{\text{out}}(x) \) is the guiding thread of this paper. For a general complex momentum \( p = z \) one directly has the so-called background solutions. For instance, out of (6) one has

\[
\Psi_e^{+r}(x) = \mathcal{N}(z) \begin{cases} 
  e^{ixx} + R(z) e^{-ixx} & , \quad x \leq 0 \\
  N^{-1} \Psi_e^{+r}(x) & , \quad 0 < x < L \\
  T(z) e^{ixx} & , \quad x \geq L 
\end{cases}
\]  

(7)

where \( \mathcal{N}(z) = \sqrt{m/\sqrt{2\pi z}} \) and \( \mathcal{E} = \frac{x^2}{2m} \) is the complex energy. We notice that, for \( z \) almost everywhere in \( \mathcal{C} \), the absolute value of (7) diverges for \( x \rightarrow +\infty \), \( x \rightarrow -\infty \), or both, because of the presence of the asymptotic reflected wave. As an example, we see that \( \Psi_e^{+r}(z; x) \) diverges for \( x \rightarrow \pm \infty \) when \( z \in \mathcal{C}_- \), and only for \( x \rightarrow -\infty \) when \( z \in \mathcal{C}_+ \).

The solution (7) features reflection, transmission (and others in the region \([0, L]\)) amplitudes, which share a common denominator \( D_+(z) \), which is related to the (radial) Jost functions in the case of the (s-wave) 3-D scattering. It goes similarly for the general solution \( \Psi_e^{+r,l}(x) \). Generally, \( D(z) \) has complex zeroes \( z = p_n \) (resonances) and pure imaginary ones \( z = p_i \) (bound and anti-bound momenta). We then write \( R = \mathcal{R}(z)/D_+(z) \), \( T = \mathcal{T}(z)/D_+(z) \), etc., where the numerators are holomorphic functions of \( z \). Multiplying (7) by \( D_+(z) \) we then define the Master Solution

\[
\Phi_e^{+r}(x) = \mathcal{N}(z) \begin{cases} 
  D_+(z) e^{ixx} + \mathcal{R}(z) e^{-ixx} & , \quad x \leq 0 \\
  N^{-1} \Phi_e^{+r}(x) & , \quad 0 < x < L \\
  T(z) e^{ixx} & , \quad x \geq L 
\end{cases}
\]  

(8)

For real \( z = p > 0 \), \( D_+(p) \) is regular and one one has \( \Phi_e^{+r}(x) = D_+(p) \psi_r^{+r}(x) \). Instead, (8) readily yields the resonant and (we shall see) anti-bound solutions, respectively at \( z = p_n \) and \( z = p_i \).

As an example, the denominator \( D_+(p) \), specific to the in states \( r, l \), and its partner \( D_-(p) \) of the out states, have the following form in the case of a square potential well with depth \( V < 0 \) and width \( L \):

\[
D_+(p) = (p + \hat{p})^2 e^{-ipL} - (p - \hat{p})^2 e^{ipL} \\
D_-(p) = (p + \hat{p})^2 e^{ipL} - (p - \hat{p})^2 e^{-ipL}
\]  

(9)

where \( \hat{p} = \sqrt{p^2 - 2mV} \). For real \( p \) they are related by complex conjugation, which is equivalent to changing the sign of the momenta \( p \rightarrow -p \), \( \hat{p} \rightarrow -\hat{p} \). Notice that the derivation of (9) from SBCs is valid only for \( \hat{p} \neq 0 \), so that the value \( \hat{p} = 0 \) (to which it corresponds \( p = p_{\pm} = \pm 1/2\sqrt{2m|V|} \) and \( E = V \)) is a meaningless zero of (9). In fact, \( p_{\pm} \) are the only points of \( \mathcal{C} \) for which no eigenfunction of (1) obeying SBCs exists, whereas \( E = 0 \) (i.e. \( p = 0 \)) is a proper eigenvalue (although \( p = 0 \) is not a zero of (9)) to which the trivial null scattering eigenfunction corresponds. For IBCs (or OBCs) the eigenfunctions corresponding to \( p_+ \) (or \( p_- \)) exist but are null.
General inner products

As noticed above, there exists a crisscrossed genetic kinship between the in (out) scattering solutions and the outgoing (incoming) resonances defined by the OBCs (IBCs), including the anti-bound (bound) states, rendering the extension of the former to the complex plane a little messy [7]. For complex momenta the terms incoming and outgoing loose much physical meaning, which maybe related, at most, to the sign of the real part of the momenta. This relationship breaks down for the resonant (either outgoing or incoming) solutions, which have momenta with both positive and negative real parts, and it is fully meaningless for the bound and anti-bound solutions, which have zero real part. The OBCs (IBCs) rather determine the location of the zeroes in $\mathcal{C}_- \ (\mathcal{C}_+)$. In fact, it can be shown (Appendix A) that the OBCs (IBCs) imply that the momenta of the solutions feature a negative (positive) imaginary part, regardless the real part being zero (bound and anti-bound states) or finite (resonances).

The zeroes of the denominators (9) can be pinpointed only by numerically computing the roots of $\mathcal{D}_+(p) = 0$ or $\mathcal{D}_-(p) = 0$. However the naive use of mathematical programs may yield spooky results that can be traced back to the default used for the branching of the Square Root function, so that $\sqrt{z^2}$ not always yields $z$. For instance, in the case of $\mathcal{D}_+ = 0$ for the square well in (9), one may find the expected resonance zeroes in $\mathcal{C}_-$ together with only part of the anti-bound momenta in the lower imaginary axis plus some bound state momenta (upper axis). The remaining ones, together with the incoming resonant momenta in $\mathcal{C}_+$, stem from $\mathcal{D}_- = 0$, the roots of which are the complex conjugates of $\mathcal{D}_+ = 0$.

To conclude this section, an overview of the location in the complex plane of the momenta corresponding to the different types of solutions above is given in Figure 1.

3. Inner products

From the MS (8) we may obtain a Master Inner Product (MIP)

$$\langle \mathcal{E}|\mathcal{E}' \rangle = \int_{-\infty}^{+\infty} dx \Phi_\mathcal{E}^*(x)\Phi_{\mathcal{E}'}(x)$$

(10)

where the labels $+, r$ are understood and will be omitted in the following. The integral can be computed along the usual lines (Appendix B), yielding

$$\langle \mathcal{E}|\mathcal{E}' \rangle = N^* N' \left\{ \begin{array}{l}
[I(z^* - z') - \frac{i}{z^* - z'}] D^* D' \\
+ [I((-z^* - z')) + \frac{i}{z^* - z'}] (R^* R' + T^* T') \\
+ [I(-(z^* + z')) + \frac{i}{z^* + z'}] R^* D' \\
+ [I(z^* + z') - \frac{i}{z^* + z'}] D^* R'
\end{array} \right\}$$

(11)

where $I(k) \equiv \int_0^\infty dx \, e^{ikx}$, and the primed notation is explained in that Appendix. All the inner products of the different families of solutions with themselves, and with each other, can be derived from (11), and in the remaining of this section we shall outline the technicalities of the most relevant cases.
3.1. Scattering states

For real \( z = p \) and \( z' = p' \), we readily see that the MIP (11) yields \(|\mathcal{D}|^2 \langle E|E'\rangle\):

\[
\langle E|E'\rangle = \mathcal{D}^* \mathcal{D}' \langle E|E'\rangle = \mathcal{D}^* \mathcal{D}' N^* N' \left\{ \begin{array}{l}
[I(p-p') - \frac{i}{p-p'}] + [I(-(p-p')) + \frac{i}{p-p'}] (R^* R' + T^* T') \\
+ [I(-(p+p')) + \frac{i}{p+p'}] R^* \\
+ [I(p+p') - \frac{i}{p+p'}] R'
\end{array} \right. (12)
\]

For real \( k \), the integrals \( I(k) \) are singular (Appendix C) and must be interpreted as a distribution, namely

\[
I(\pm k) = \pm i \text{PV} \frac{1}{k} + \pi \delta(k) \quad (13)
\]

As a result, all the terms proportional to \((p \pm p')^{-1}\) stemming from these Principal Values, plus the ones displayed in (12), cancel out. The terms \( \delta(p+p') \) vanish because \( p+p' \) is always \( > 0 \), and the terms \( \delta(p-p') \) sum up to

\[
\langle E|E'\rangle = \frac{1}{2\pi \sqrt{pp'}} \pi \delta(p-p') [1 + |R|^2 + |T|^2] = \frac{m}{p} \delta(p-p') = \delta(E-E') \quad (14)
\]

as expected from the wave function normalization adopted.

3.2. Background states

For general complex \( z \) and \( z' \), the general form of \( I(k) \) (Appendix C) leads to the result

\[
\langle \mathcal{E}|\mathcal{E}'\rangle = \left\{ \begin{array}{l}
0 \quad , \quad -\frac{\pi}{4} < \arg(z' - z^*) < \frac{5\pi}{4} \\
\infty \quad , \quad \text{otherwise}
\end{array} \right. (15)
\]

Thus, for each background state \( |\mathcal{E}\rangle \) of momentum \( z \), there is a "neighborhood of divergence" so that \( |\mathcal{E}\rangle \) is orthogonal to any other \( |\mathcal{E}'\rangle \) the momentum \( z' \) of which lies outside a "divergence wedge", with an angle of \( \pi/4 \) and apex in \( z^* \), and gives a divergent inner product if \( z' \) lies inside this wedge. The rule is reciprocal: we may consider as well the location of \( z \) with respect to the wedge with apex in \( z'^* \). In particular \( \langle \mathcal{E}|\mathcal{E}\rangle = \infty \), as expected. When both \( z \) and \( z' \) lie on the real axis, both apexes fall on the real axis so that the only divergent products happens for \( z = z' \), as already known for the scattering states.

The products with other states yield highly variable results depending on the location of \( z \) on the whole complex plane. Of most interest is the sector \( 7\frac{\pi}{4} < \arg(z) < 2\pi \), in which case the states \( |\mathcal{E}\rangle \) are orthogonal to the bound states and partially orthogonal to the anti-bound and to the scattering states.

3.3. Bound and Anti-bound states

As explained in 2.4., the MS (8) stems from the analytical continuation of the scattering \( in \) solutions we are mainly considering. Then the zeroes of \( \mathcal{D}_+(z) \) lie only in \( \mathcal{C}_- \) and do not include the bound state momenta. However, apart from the specific form of the amplitudes \( R \) and \( T \), both bound (which would stem from the scattering \( out \) solutions,
then corresponding to zeroes of \( \mathcal{D}_-(z) \), lying in \( \mathcal{C}_+ \) and anti-bound solutions share the general form (8) with respectively \( \mathcal{D}_+ = 0 \). For ease of writing, in this subsection we drop the tilde notation introduced in 2.1. Thus we consider bound states \( |\phi_i| \) with purely imaginary momenta \( z_i = iq_i (q_i > 0) \), while the anti-bound states have \( q_i < 0 \). The general inner products \( \langle \phi_i | \phi_j \rangle \) stem from (11) with the simplification \( \mathcal{D} = \mathcal{D}' = 0 \).

The bound states involve only finite integrals. For \( i \neq j \) we have

\[
\langle \phi_i | \phi_j \rangle = \frac{1}{2\pi} \frac{m}{\sqrt{q_i q_j}} (R_i^* R_j + T_i^* T_j) \left[ I(i(q_i + q_j)) - \frac{1}{q_i + q_j} \right] = 0
\]  

since

\[
I(i(q_i + q_j)) = \int_0^\infty dx e^{-(q_i + q_j)x} = \frac{1}{q_i + q_j}
\]  

It is instructive to notice that (B.3) becomes

\[
-(q_i^2 - q_j^2) \int_0^L dx \phi_i^* \phi_j = 2m(E_i - E_j) \int_0^L dx \phi_i^* \phi_j
\]

\[
= W[\phi_i^*, \phi_j]_0^L = (q_i - q_j) \frac{1}{2\pi} \frac{m}{\sqrt{q_i q_j}^2} (R_i^* R_j + T_i^* T_j e^{-(q_i + q_j)L})
\]

and (B.4) now is

\[
\int_0^L dx \phi_i^* \phi_j = -\frac{1}{(q_i + q_j)} \frac{1}{2\pi} \frac{m}{\sqrt{q_i q_j}^2} (R_i^* R_j + T_i^* T_j e^{-(q_i + q_j)L})
\]

For \( i = j \), (18) is useless for the calculation of \( \int_0^L dx \phi_i^* \phi_i \). Instead the (finite) norm \( \|\phi_i\|^2 = \langle \phi_i | \phi_i \rangle \) can be obtained by using the Wronskian \( W[\phi_i^*, \partial_q \phi_i] \) (see [9] for this "method of quadratures", say integration by parts, applied to resonances). Noticing that \( \partial_x^2 \phi_i = [2mV(x) + q_i^2] \phi_i \) and that \( \partial_x^2 \partial_q \phi_i = [2mV(x) + q_i^2] \partial_q \phi_i + 2q_i \phi_i \), we now have

\[
2q_i \int_0^L dx \phi_i^* \phi_i = W[\phi_i^*, \partial_q \phi_i]_0^L
\]

On the other hand, using the BCs at \( x = 0, L \), the terms involving the derivatives \( \partial_q \mathcal{R}_i \) and \( \partial_q \mathcal{T}_i \) cancel out so that we now have

\[
W[\phi_i^*, \partial_q \phi_i]_0^L = \frac{1}{2\pi} \frac{m}{q_i} (|\mathcal{R}_i|^2 + |\mathcal{T}_i|^2 e^{-2q_i L})
\]

and hence

\[
\int_0^L dx \phi_i^* \phi_i = \frac{1}{2\pi} \frac{m}{2q_i^2} (|\mathcal{R}_i|^2 + |\mathcal{T}_i|^2 e^{-2q_i L})
\]

(notice that the inadvertent use of (19) with \( i = j \) yields (22) albeit for a crucial global sign). Then

\[
\langle \phi_i | \phi_i \rangle = \frac{1}{2\pi} \frac{m}{q_i} (|\mathcal{R}_i|^2 + |\mathcal{T}_i|^2) \int_0^\infty dx e^{-2q_i x} \int_0^L dx e^{2q_i x} + \int_0^L dx \phi_i^* \phi_i
\]

\[
= \frac{1}{2\pi} \frac{m}{2q_i^2} (|\mathcal{R}_i|^2 + |\mathcal{T}_i|^2 e^{-2q_i L}) + \int_0^L dx \phi_i^* \phi_i
\]

\[
= \frac{1}{2\pi} \frac{m}{q_i^2} (|\mathcal{R}_i|^2 + |\mathcal{T}_i|^2 e^{-2q_i L})
\]

(23)
which yields the wave function normalization factor needed for having \( \langle \phi_i | \phi_j \rangle = \delta_{ij} \).

The inner products of the anti-bound states between themselves are divergent, as expected. However, their products with the bound states are dominated in some cases by the convergent spatial behaviour of the latter, in which case we have orthogonality. From (17) we see that this happens whenever \((q_i + q_j) > 0\), the integral being divergent otherwise.

Likewise, the convergent power of the bound states may dominate over the divergent behaviour of the general background solutions, so that a partial “wedge” orthogonality governs also these crossed inner products.

The textbook orthogonality between the bound and the scattering states can be immediately read out from (11). For the product \( \langle \phi_i | E \rangle \) one has \( \mathcal{D} = 0 \), the integrals \( I(iq_i \pm p) \) are finite and yield \( i(q_i \pm p)^{-1} \) respectively, so that we have \( \langle \phi_i | E \rangle = 0 \).

### 3.4. Resonant and Scattering states

Consider a resonance with momentum \( p_n \) and a scattering in state with real momentum \( p > 0 \). Omitting an irrelevant normalization factor \( N_n^* N \), then (11) reduces to

\[
\langle z_n | E \rangle \propto \left[ I(-(p_n^* - p)) + \frac{i}{p_n^* - p} \right] (\mathcal{R}_n^* \mathcal{R} + \mathcal{T}_n^* \mathcal{T}) + \left[ I(-(p_n^* + p)) + \frac{i}{p_n^* + p} \right] \mathcal{R}_n^* \mathcal{D}(p) \tag{24}
\]

With \( p > 0 \), for \( n > 0 \) we always have \(-\frac{\pi}{4} < \arg(-(p_n^* + p)) < \frac{5\pi}{4}\), so that

\[
\langle z_n | E \rangle \propto \left[ I(-(p_n^* - p)) + \frac{i}{p_n^* - p} \right] (\mathcal{R}_n^* \mathcal{R} + \mathcal{T}_n^* \mathcal{T}) \tag{25}
\]

and therefore, with the prescription adopted,

\[
\langle z_n | E \rangle = \begin{cases} 0 & \text{if} \ -\frac{\pi}{4} < \arg(p - p_n^*) < \frac{5\pi}{4} \\ \infty & \text{otherwise} \end{cases} \tag{26}
\]

This means that a given scattering in state \( | E \rangle \) (with momentum \( p > 0 \) on the real axis) is orthogonal to any \( | z_n \rangle \) (with \( n > 0 \)) if the momentum \( p_n \) lies outside the wedge with apex in \( p \), the inner product being divergent otherwise. Viceversa, given \( p_n \), the momenta \( p \) of the orthogonal scattering states lie outside the wedge with apex in \( p_n \).

The scattering states have a reflected wave with momentum of opposite sign to the incident one, so the situation is trickier for \( n < 0 \). Given \( p_{-|n|} \), the wedge to be considered is again the one with apex in the mirror momentum \( p_{|n|} \).

### 3.5. Resonant and bound states

Up to a normalization factor, the MIP now reduces to

\[
\langle \phi_i | z_n \rangle \propto (\mathcal{R}_n^* \mathcal{R} + \mathcal{T}_n^* \mathcal{T}) [I(iq_i + p_n) - \frac{i}{iq_i + p_n}] \tag{27}
\]

The integral is convergent, yielding \( i(q_i + p_n)^{-1} \) and hence \( \langle \phi_i | z_n \rangle = 0 \), provided that \( q_i > |\text{Im} p_n| \). We thus have a situation similar to that occurring between resonances, namely that the states are orthogonal if the bound state momentum, lying in the positive imaginary axis, and the resonant one, lie outside the respective divergence wedges, the
inner product being infinite otherwise. For a potential well of finite depth featuring both bound and resonant states, the latter case happens only for a few of the (finite number of) bound states.

3.6. Resonances and anti-bound states

As long as we start from the solution (8), which satisfies an OBC, and from the corresponding MIP (11), in this subsection we consider the inner products of the states with isolated momenta lying in the lower half complex plane, namely the outgoing resonances with themselves and with the anti-bound solutions. The result is similar to (15), albeit for the fact that the momenta \( z \) and \( z' \) take the isolated denumerable values \( iq_i \) or \( z_n \):

\[
\langle a | b \rangle = \begin{cases} 
0 & \frac{-\pi}{4} < \arg(z_b - z_a^*) < \frac{5\pi}{4} \\
\infty & \text{otherwise} 
\end{cases}
\]

where the labels \( a \) and \( b \) run over the the values of \( i \) or \( n \). A similar layout of "divergence wedges" comes out.

Through this section the structure of divergence wedges above describes a partial orthogonality between the members of the different families of solutions of the SE. We shall call it "wedge orthogonality" and indicate it by the symbol \( \Delta_{ab} \). In the Figure 1 we have depicted the divergence wedge of the resonant state \(|z_2\rangle\). Examples involving resonant and scattering solutions can be found in Figure 2 in [4].

![Figure 1](image.png)

**Figure 1.** Location of the momenta of the solutions.

Two bound states are assumed. An example of "wedge orthogonality" is given between resonant states: \( \langle z_2 | z_n \rangle = 0 \) for \( n < 0 \) and \( n > 4 \), while \( \langle z_2 | z_m \rangle = \infty \) for \( 0 < m \leq 4 \).
3.7. General products

All the inner products considered above may be displayed in the following comprehensive table:

|   | \(\langle a | b \rangle\) | \(\langle \phi_2 | \phi_1 \rangle\) | \(\langle \phi_{1'} | \phi_{2'} \rangle\) | \(\langle z_n | \tilde{z}_m \rangle\) | \(\langle E | E' \rangle\) | \(\langle \mathcal{E}' \rangle\) |
|---|---|---|---|---|---|---|
| \(\langle \phi_2 \rangle\) | 1 | 0 | \(\infty\) | 0 | 0 | 0 | \(\Delta_{ab}\) |
| \(\langle \phi_1 \rangle\) | 0 | 1 | \(\infty\) | \(\infty\) | 0 | 0 | \(\Delta_{ab}\) |
| \(\langle \phi_{1'} \rangle\) | 0 | \(\infty\) | \(\infty\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) |
| \(\langle \phi_{2'} \rangle\) | \(\infty\) | \(\infty\) | \(\infty\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) |
| \(\langle z_n \rangle\) | 0 | 0 | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | 0 | \(\Delta_{ab}\) | \(\Delta_{ab}\) |
| \(\langle \tilde{z}_m \rangle\) | 0 | 0 | \(\Delta_{ab}\) | \(\Delta_{ab}\) | 0 | \(\Delta_{ab}\) | 0 | \(\Delta_{ab}\) |
| \(\langle E \rangle\) | 0 | 0 | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | 0 | \(\delta(E - E')\) | \(\Delta_{ab}\) |
| \(\langle \mathcal{E} \rangle\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) | \(\Delta_{ab}\) |

Here a barrier including a well of finite depth supporting two ordinary bound states \(|\phi_1\rangle\) and \(|\phi_2\rangle\) with energies \(|E_1| < |E_2|\), plus the mirror anti-bound states \(|\phi_{1'}\rangle\) and \(|\phi_{2'}\rangle\), has been assumed, with the ordering \(q_2 > q_1 > 0 > q_{1'} > q_{2'}\). The value of the products involving the background states \(|\mathcal{E}\rangle\) depends on their momentum \(z\), the range of which is the whole \(\mathcal{C}\). Here we have considered \(z\) and \(z'\) in \(\mathcal{C}_-\).

4. Conclusions

We have calculated the relevant inner products involving the resonant eigenstates and the more general complex energy ”background” solutions in the example of a 1-dimensional quantum potential barrier with compact support. As it is well known, these states respectively have discrete and continuum complex energies and, in the space spanned by them, the Hamiltonian is not Hermitian, so that the usual neat results about the (either Dirac or Kronecker-\(\delta\)) orthogonality, the reality of the norms, etc., do not hold. On the other hand, their modulus grows exponentially at the spatial infinity, giving rise to infinite norms and seemingly infinite inner products.

Among the variety of proposals to circumvent these difficulties, we have adopted a Gaussian convergence factor, first introduced by Zel’dovich, and carried out the limit of the integrals where the factor fades off to unity. This prescription yields inner products such that most of these states are orthogonal to each other, except when they lie in a neighborhood described by a ”divergence wedge” in the complex-momentum plane, in which case the product is infinite.

The guiding thread of this paper relies on the analytic continuation to the momentum complex plane \(\mathcal{C}\) of the scattering solutions. In doing so, we have started from an \(in\), right-moving, solution (obeying an Outgoing Scattering Boundary Condition), from which a Master Solution is obtained. This MS describes the whole family of solutions when the momentum takes particular values in \(\mathcal{C}\), namely the (\(in, r\)) scattering states for \(z = p \in \mathcal{R}_+\), the anti-bound states for isolated \(z_i \in \mathcal{I}_-\), the outgoing resonances (obeying two Outgoing BCs) for isolated \(z_n \in \mathcal{C}_-\), and the
continuum of the general background solutions which are holomorphic in the remaining
of $C$. An alternative MS can be defined starting from the out scattering states (obeying
an Incoming Scattering BC), which gives rise to the bound states and to the incoming
resonances (obeying two Incoming BCs), all of them with momenta $\in C_+$. An important result is that the outgoing (incoming) BCs dictate that the solution’s
momenta $\in C_-$ ($\in C_+$) in full generality, that is regardless their real part being finite
(resonances) or null (anti-bound or bound states). This makes the outgoing resonances
akin to the anti-bound states (and the incoming ones to the bound states), whereas
there is a somehow messy crossed kinship between the outgoing (incoming) BCs and
the parent in (out) MS.

Out of the MS above a Master Inner Product has been defined, from which all
the inner products between the members of the different families of solutions stem.
Generally a partial “wedge orthogonality” is obtained, which we denote by the symbol
$\Delta_{ab}$, from which the expected infinite norms of all the solutions, except for the bound
states, results. Of course, the traditional orthogonality relations between the (real
energy) bound and scattering states, namely the Kronecker-\(\delta\) and the Dirac-\(\delta\), arise as
particular cases. This results is different from the full bi-orthogonality obtained by the
prescription of analytically continuing the finite integrals from $C_+$ to the whole $C_-$,
where the integrals are formally divergent. Our limiting procedure instead extends the
finite result to only the $\pi/4$ wedges of $C_-$ close to the real axis.

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Appendix A. Boundary conditions and pole location

We work out the relationship between the OBCs, the IBCs, and the location of the
momenta in the complex plane. We first re-derive for 1-D quantum systems the known
link between the OBCs and the resonances in the lower half plane [6] [8].

We re-write (1) in the more convenient form

$$\partial_x^2 u(x) = [2mV(x) - p^2] u(x)$$

(A.1)

and consider the OBCs (4) together with their complex conjugates. Computing the
expression

$$\int_0^L dx \left[ u^* \partial_x^2 u - u \partial_x^2 u^* \right]$$

(A.2)

both using (A.1) and integration by parts, yields the equality

$$(p^*^2 - p^2) \int_0^L dx \ |u|^2 = i(p + p^*)(|u(0)|^2 + |u(L)|^2)$$

(A.3)
With $p = \alpha + i\beta$ one obtains

$$-i4\alpha\beta \int_0^L dx\ |u|^2 = i2\alpha(|u(0)|^2 + |u(L)|^2),$$

(A.4)

which, for $\alpha \neq 0$, yields

$$\beta = -\frac{|u(0)|^2 + |u(L)|^2}{2\int_0^L dx\ |u|^2} < 0.$$ (A.5)

The case $\alpha = 0$ (anti-bound solutions) may be dealt with by using the momentum-derivative $u'(x) \equiv \partial_x u(x)$, which obeys the equations $\partial^2_x u' = [2mV - p^2] u' - 2p u$ and $\partial_x u'|_0 = -i p u'(0) - i u(0), \partial_x u'|_L = i p u'(L) + i u(L)$, and starting from the expression

$$\int_0^L dx\ [u^* \partial^2_x u' - u' \partial^2_x u^*].$$ (A.6)

Then we obtain the equality

$$-i4\alpha\beta \int_0^L dx\ u^* u' - 2(\alpha + i\beta) \int_0^L dx\ |u|^2$$

$$= i2\alpha(u^*(0)u'(0) + u^*(L)u'(L)) + i(|u(0)|^2 + |u(L)|^2)$$

(A.7)

which, for $\alpha = 0$, yields the same result (A.5).

The IBCs lead to $\beta > 0$ for any $\alpha$, and give rise to both the incoming resonances and the bound states.

**Appendix B. Master Inner Product**

The space integral in (10) can be split in three sectors

$$\langle E|E'\rangle = N^*N'$$

$$\left\{ \begin{array}{l}
\int_0^\infty dx\ [D^*D'Ie^{-i(z^*-z')x} + R^*R'e^{i(z^*-z')x} \\
+ R^*D'e^{i(z^*+z')x} + D^*R'e^{-i(z^*+z')x}] \\
+(N^*N')^{-1} \int_0^L dx\ \Phi^*_E(x)\Phi_{E'}(x) \\
+ \int_0^L dx\ \Phi^*_E(x)\Phi_{E'}(x)
\end{array} \right.$$ (B.1)

with the short-hand notation $N^* \equiv (N(z))^*, N' \equiv N(z')$, and similarly for $D$ and the amplitudes $R$ and $T$. We then bring all the infinite-limited integrals to the form $I(k) = \int_0^\infty dx\ e^{ikx}$, so that

$$\langle E|E'\rangle = N^*N'$$

$$\left\{ \begin{array}{l}
I(z^* - z')D^*D' + I(-z^* + z')(R^*R' + T^*T') \\
+ I(-z^* + z')D^*R' + I(z^* + z')D^*R' \\
+(N^*N')^{-1} \int_0^L dx\ \Phi^*_E(x)\Phi_{E'}(x) \\
- T^*T' \int_0^L dx\ e^{-i(z^* - z')x}
\end{array} \right.$$ (B.2)

The form (8) of the solution at $x = 0$ and at $x = L$ lets expressing $\int_0^L dx\ \Phi^*_E\Phi_{E'}$ in terms of the amplitudes $D, R$ and $T$ outside the barrier. The procedure uses the operator $\partial^2_x$ for which $\partial^2_x \Phi_E = 2m(V - E)\Phi_E$, and integration by parts to obtain

$$(z^2 - z'^2) \int_0^L dx\ \Phi^*_E\Phi_{E'} = 2m(E^* - E') \int_0^L dx\ \Phi^*_E\Phi_{E'}$$

$$= \int_0^L dx\ \Phi^*_E(x)(\partial^2_x - \partial^2_x)\Phi_{E'}(x) = \left[\Phi^*_E, \Phi_{E'}\right]_0^L$$

$$= i(z^* + z')N^*N'(-D^*D' + R^*R' + T^*T'e^{-i(z^* - z')L})$$

$$+ i(z^* - z')N^*N'(R^*D' - D^*R'),$$ (B.3)
where $W[\phi, \psi] \equiv \phi \partial_x \psi - \psi \partial_x \phi$ is the Wronskian, so that
\[
\int_0^L dx \, \Phi^*_E \Phi_{E'} = \frac{iN^* N'}{z^* - z'}(-D^* D' + R^* R' + T^* T' e^{-i(z^* - z')L}) + \frac{iN^* N'}{z^* + z'}(R^* D' - D^* R')(B.4)
\]
provided that $E^* \neq E'$ (i.e. $z^{*2} \neq z'^2$). The finite last integral term in (B.2) gives the result $i(z^* - z')^{-1}T^* T'(1 - e^{-i(z^* - z')L})$, which readily leads to (11).

The case $E^* = E'$ arises in the calculation of the norms whether they be finite (bound states) or divergent (all the others). In the latter case, the infinite result shows up already in the integrals $I(k)$ in (B.2), regardless of the method used to compute the finite integral $\int_0^L dx \, \Phi^*_E(x) \Phi_{E'}(x)$. We calculate the finite result of the bound states in 3.3 by using the technique of quadratures.

### Appendix C. Infinite-limited integrals

For computing $I(k)$ we rely on the limit $\lambda \to 0$ of the basic Gaussian regularized integral
\[
J(k, \lambda) \equiv \int_0^{+\infty} dx \, e^{-\lambda x^2} e^{i k x} = \frac{i}{k} \sqrt{\pi/\tau} e^{\tau^2} \text{erfc}(\tau) \quad (\lambda \text{ real } > 0)
\]
which is directly related to (7.1.2) in [10], where $\tau = -i k / (2\sqrt{\lambda})$, and hence $k$, can take any complex value. See Appendix A in [4] for more details.

For $\text{Im} k > 0$ the integral is always convergent so that the limit can be taken in the integrand in (C.1). Then we trivially have $I(k) \equiv J(k, 0) = i k^{-1}$.

For real $k$, the quoted result
\[
\int_0^{\infty} dx \, e^{i k x} = i PV \frac{1}{k} + \pi \delta(k)
\]
relies on adding to $k$ a small imaginary part $i \epsilon$, which still guarantees the convergence when $\lambda \to 0$, but later in the limit $\epsilon \to 0_+$ the result must be interpreted as a distribution.

For $\text{Im} k < 0$ the integration and the limit $\lambda \to 0$ do not commute and we adopt the limit of the integral as a prescription. From (7.1.23) in [10] we obtain
\[
I(k) \equiv J(k, 0) = \begin{cases} \frac{i}{k} \infty, & -\frac{\pi}{4} < \arg(k) < \frac{5\pi}{4}, \quad k \neq 0 \\ \infty, & \text{otherwise} \end{cases}
\]
which extends the finite result $i k^{-1}$ to a new region of $C_-$ and defines the ”divergence wedge” there mentioned.

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