Scattering in PT-symmetric Quantum Mechanics

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- **Summary**

- After a brief prelude concerning my relation to Sandro Graffi, I discuss scattering in PT-symmetric one-dimensional quantum mechanics within the Schrödinger and Dirac framework.

- In addition to standard local finite-range potentials also non-local separable potentials will be considered.
My relation to Graffi may be encapsulated in two dates:
*I met him first in 1966*
The first hint may be that I was assigned by Graffi a problem which took me 40 years to solve and finally I got the solution helped by Caliceti: in the following I will give an alternative explanation though the crucial role of Caliceti to convert a possibly virtual into a real effective collaboration should not be underestimated.
As a third year student of quantum theory of matter I met Sandro Graffi in the academic year 1966-1967 when he was graduating in theoretical physics supervised by Prof. F. Selleri, also G. Turchetti and V. Grecchi belonged to the same team. The scientific interest of Prof. Selleri focused on particle physics phenomenology with a prevailing role of creative enthusiasm over sound but less exciting analytic accuracy. Anyway 68 was coming soon, it already started so to speak in 67. Prof. Selleri was deeply affected and together with many theoretical physicists turned left. In their minds science and political ideologies got superposed, slightly more sophisticated (involving possible complexity) than mixed up.
• Thereby I mean that the emphasis was to show that Quantum Mechanics had problems and some very essential concepts like entanglement were scrutinized.

• Because of the trend, however (superposition of Quantum Mechanics and ideology) some consequences like quantum information theory which could have been grasped at that time were not unveiled. Lost opportunity!
• One cannot deny that those were exciting days. As a student I was confronted with the conundrums of Quantum Mechanics and Graffi and Grecchi helped me to understand the loopholes of some paradoxes. The prevailing revolutionary trend was to consider Quantum Mechanics as a kind of idealistic science to be superseded by a more materialistic one since Marxism was a kind of TOE, Theory Of Everything. Correspondingly the interest of Prof. Selleri drifted from particle physics phenomenology to the foundations of Quantum Mechanics, with the intention to falsify it in the spirit of Popper.
Graffi and his team mates Grecchi and Turchetti were shrewd enough to grasp that for young physicists it was a trap to get involved in such topics, so they tried quickly to become independent and master of their scientific research. They did not encourage me to graduate with Prof. Selleri. They moved to Mathematical Physics and I moved to Theoretical Nuclear Physics with the idea that these latter fields might be less exciting but people knew better what they were talking about. So here there is a very good reason why INFN should support Graffi's celebration: in Bologna nothing like a Sakata school or a Vigier-DeBroglie school was built with the associated risks typical of a dogmatic top down approach.
At that time Graffi and Grecchi got a job in INFN as young researchers: INFN was a flexible and informal institution promoting mainly particle physics but also related fields of research; it provided financial support to university research (like NSF so to speak) but also gave the opportunity to hire full time physicists, engineers and technicians. For physicists these jobs were not intended to become permanent: the reason was that in a physicist's career it was thought to be effective to work few years in research full time and after that to be hired in university.
This precisely occurred to Graffi and Grecchi and as soon as they got jobs at university I was ready for INFN (where I still keep my job since in later times the INFN →University transition became much more cumbersome at least for theoretical physicists in Bologna). Since our scientific interests diverged I was less than superficially aware of what Graffi was doing until again in 1997-98 my research in SUSYQM intersected inadvertently earlier research by Caliceti Graffi and Maioli(1980). SUSYQM lead Andrianov, Ioffe, Junker, Trost and myself to consider isospectrality between non hermitian hamiltonians and hermitian ones, introducing a partnership between Schrödinger operators with real potentials and spectrum and Schroedinger operators with specific complex potentials.
It took however few years before I realized there was a connection with Caliceti et al and that occurred only after few years of flourishing PT symmetric Quantum Mechanics, actually it was M.Znojil visiting us in 2000 to promote our awareness of each other's results. Graffi is still associated to INFN as an external collaborator belonging to the INFN theory group and his reputation and his activity is certainly crucial for the developments of mathematical physics in Bologna thus this is a second very good reason for INFN to support the celebration. Finally let me thank the organizers for providing the opportunity to recall Graffi's very early INFN research.
I will not touch any fundamental physical interpretation of PT symmetric Quantum Mechanics in the sense of foundations of Quantum Mechanics.

In particular I will refer to one dimensional problems, so the potential will be symmetric under change of sign of the coordinate combined with complex conjugation.

The conventional wisdom is that these Hamiltonians are representative of dynamical systems which are not isolated, though loss of hermiticity occurs in a very peculiar way.
There are particular cases when there is a similarity transformation between these Hamiltonians and hermitian operators (PT-symmetric Hamiltonians have real spectrum in this case) but the hermitian operators may not be of Schrödinger type, i.e. kinetic term plus local potential. I will focus attention on scattering properties of PT symmetric Hamiltonians. My research in this field has been carried out mainly with Alberto Ventura from ENEA. Those which will not appreciate non-hermitian Hamiltonians may tentatively think that we are dealing with problems in optics with a complex index of refraction characterized by handedness.
This interpretation is made possible by the close relation of the stationary Schrödinger equation to the classical Helmholtz equation. Later on we will extend our discussion to non local potentials enjoying PT symmetry considering separable kernels of the type

\[ K(x,y) = g(x) \cdot h(y) \cdot \exp(iax) \cdot \exp(iby) \]

with \( g \) and \( h \) real even functions of their arguments and \( a \) and \( b \) real constants. PT symmetry of separable \( K(x,y) \) appears rather natural.
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• One-dimensional Schrödinger equation for a monochromatic wave of energy $E = k^2$ scattered by a non-local potential with kernel $K$ in units $\hbar=2m=1$:

  \[-(d^2/dx^2) \Psi(x) + \lambda \int K(x,y) \Psi(y) dy = k^2 \Psi(x)\]

• where $\lambda$ is real and $K$ is separable:

  \[K(x,y) = g(x) \cdot h(y) \cdot \exp(iax) \cdot \exp(iby)\]

• ($a$ and $b$ real, $g$ and $h$ real functions vanishing at $\pm\infty$)

• Hermiticity: $K(x,y) = K^*(y,x)$

• $P$ invariance: $K(x,y) = K(-x,-y)$

• $T$ invariance: $K(x,y) = K^*(x,y)$

• $PT$ invariance: $K(x,y) = K^*(-x,-y)$
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<table>
<thead>
<tr>
<th>Property</th>
<th>Condition</th>
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<tbody>
<tr>
<td>Reality</td>
<td>$a = b = 0$</td>
</tr>
<tr>
<td>Symmetry under $x \leftrightarrow y$</td>
<td>$a = b, \ g = h$</td>
</tr>
<tr>
<td>Hermiticity</td>
<td>$a = -b, \ g = h$</td>
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<tr>
<td>P invariance</td>
<td>$a = b = 0, \ g(x) = g(-x), \ h(y) = h(-y)$</td>
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<tr>
<td>T Invariance</td>
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Finally we provide the PT symmetric scenario for the one dimensional Dirac equation. Again those who do not like complex potentials in a Dirac equation may think of a suitable Dirac-like behaviour of a non relativistic tight binding hamiltonian in one dimension for sufficiently large wave lengths, in this last scenario complex PT symmetric interactions may become more palatable. The first nearest neighbour approximation and use of the LCAO (linear combination of atomic orbitals) wave function is a crucial step to obtain Dirac-like behaviour.
We will ignore what all this means for the system mapped by the similarity transformation when this transformation exists, just because crudely speaking the mapped system may not be of Schrödinger type and furthermore the finite range or short range potential may not be mapped in a potential with the same properties. In addition from the point of view of wave functions in general there is no reason why wave functions which asymptotically behave as $e^{-ax}$, for $x = +\infty$ and $e^{+ax}$ for $x = -\infty$, $a>0$, should be mapped into ones with the same behaviour, similar considerations for wave functions behaving asymptotically as $e^{ikx}$ or $e^{-ikx}$. In order to be able to have a decent framework for scattering for the mapped system one should have for the latter continuum eigenfunctions which asymptotically can be written as superposition of such plane waves.
• The main point worrying the experts in the field is that there is a non-local effect, i.e. that the similarity transformation can affect the wave functions very far from the potential region even asymptotically when the potential is of finite range, or even zero range (Dirac delta function). This is a kind of classical prejudice!
It would be sufficient somehow to require that the similarity maps bound states into bound states and scattering states (superposition of progressive and regressive plane waves) into scattering states. To my knowledge such a detailed analysis has not been carried through. Let me recall that the similarity transformation induced by pseudohermiticity depends itself on the potential so the problem is a fully dynamical one.

A kind of rather simple similarity transformation (canonical transformation) which is not dynamical and satisfies the requirements that plane waves go to plane waves and exponentially damped waves go to exponentially damped waves is a global "small" coordinate shift. The kinetic energy does not change whereas if a real potential is originally parity invariant it will now become PT invariant.
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• L-R Representation
• General time-dependent Schrödinger equation
  • \(-\left(\frac{\partial^2}{\partial x^2}\right) \psi(x,t) + \int K(x,y) \psi(y,t) dy = i \left(\frac{\partial}{\partial t}\right) \psi(x,t)\) (1)
• written in units \(\hbar = 2m = 1\). For a monochromatic wave of energy \(\omega\) the time dependence of the wave function is
  • \(\psi(x,t) = \Psi(x)e^{-i\omega t}\) (2)
• Unless explicitly stated, we consider local potentials :
  • \(K(x,y) = \delta(x-y)V(y)\) (3)
• If Eqs. (2-3) hold, Eq. (1) reduces to
  • \(H\Psi(x) = \left(-\frac{d^2}{dx^2} + V(x)\right)\Psi(x) = k^2\Psi(x)\) (4)
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• With $k = \sqrt{\omega}$ ($> 0$) the wave number. It is convenient to work in a two-dimensional Hilbert space where the basis vectors are the kets $|R>$ and $|L>$ (and the corresponding bras $<R|$ and $<L|$). In configuration space, with the choice of the time dependent phase given in Eq. (2), $<x|R,k> \sim e^{ikx}$ represents a plane wave travelling from left to right ($L \rightarrow R$) and $<x|L,k> \sim e^{-ikx}$ a wave travelling from right to left ($R \rightarrow L$).

• In the case of a finite-range local potential, Eq. (4) admits the general solution $\Psi(x) = \alpha F_1(x) + \beta F_2(x)$, where the linearly independent solutions $F_1(x)$ and $F_2(x)$ are both of the asymptotic form...
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- \( \lim_{x \to \pm \infty} F_m(x) = a_m e^{ikx} + b_m e^{-ikx} \quad (m = 1, 2) \)

- The transmission and reflection coefficients of a progressive wave are
  - \( T_{L \to R} = \frac{(a_2 b_1 - a_1 b_2)}{(a_2 b_1 - a_1 b_2)} \)
  - \( R_{L \to R} = \frac{(b_1 b_2 - b_1 b_2)}{(a_2 b_1 - a_1 b_2)} \)

- The transmission and reflection coefficients of a regressive wave are
  - \( T_{R \to L} = \frac{(a_2 b_1 - a_1 b_2)}{(a_2 b_1 - a_1 b_2)} \)
  - \( R_{R \to L} = \frac{(a_1 a_2 - a_1 a_2)}{(a_2 b_1 - a_1 b_2)} \)
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- Equipped with $T$ and $R$ coefficients we can find two kinds of (linearly independent) wave functions $\Psi_1(x)$ and $\Psi_2(x)$, whose asymptotic forms, neglecting a global normalization factor, are
  - $\Psi_1(x) \sim e^{ikx} + R_{L \rightarrow R} e^{-ikx}$, $x \rightarrow -\infty$
  - $\sim T_{L \rightarrow R} e^{ikx}$, $x \rightarrow +\infty$

- and
  - $\Psi_2(x) \sim T_{R \rightarrow L} e^{ikx}$, $x \rightarrow -\infty$
  - $\sim e^{-ikx} + R_{R \rightarrow L} e^{ikx}$, $x \rightarrow +\infty$

- The Wronskian of $\Psi_1(x)$ and $\Psi_2(x)$ is
  - $W(x) = \Psi_1(x)d\Psi_2(x)/dx - \Psi_2(x)d\Psi_1(x)/dx$
We readily obtain $W(-\infty) = -2ikT_{R\to L}$ and $W(+\infty) = -2ikT_{L\to R}$. Thus, a necessary condition for the Wronskian to be constant on the $x$ axis is $T_{R\to L} = T_{L\to R}$.

It is easy to check that $dW/dx = 0$ for any well-behaved local potential. Therefore, the equality of the two transmission coefficients is satisfied for any such potential.
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• **P Invariance**
  – Parity invariance of the Hamiltonian $H$ implies
    • $T_{L \rightarrow R} = T_{R \rightarrow L}$ and $R_{L \rightarrow R} = R_{R \rightarrow L}$

• **T invariance**
  • Time reversal invariance of $H$ implies
    • $T_{L \rightarrow R} T^*_{R \rightarrow L} + |R_{L \rightarrow R}|^2 = 1$
    • $|R_{L \rightarrow R}| = |R_{R \rightarrow L}|$
Introducing the scattering matrix

\[ S = \begin{pmatrix} S_{RR} & S_{RL} \\ S_{LR} & S_{LL} \end{pmatrix} = \begin{pmatrix} T_{L \rightarrow R} & R_{R \rightarrow L} \\ R_{L \rightarrow R} & T_{R \rightarrow L} \end{pmatrix} \]
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• Similarity which maps plane waves into plane waves

\[ \zeta F_m = \tilde{a}_{m\pm} e^{ikx} + \tilde{b}_{m\pm} e^{-ikx} \]

• where

\[ \zeta = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \Rightarrow \zeta \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \tilde{a} \\ \tilde{b} \end{pmatrix} \]
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Transmission and reflection coefficients get linearly combined. For small complex shift translation $\zeta$ is diagonal!

$$S = \begin{pmatrix} S_{RR} & S_{RL} \\ S_{LR} & S_{LL} \end{pmatrix} \implies \tilde{S}^T = \zeta S^T \zeta^{-1}$$
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- PT invariance implies
  - \( S^I = S^* \)

- This yields for the \( S \)-matrix elements:
  - \( S_{RL} + S_{RL}^* \det S = 0 \)
  - \( S_{LR} + S_{LR}^* \det S = 0 \)
  - \( S_{LL} = S_{RR}^* \det S \)
  - \( S_{RR} = S_{LL}^* \det S \)

- This imposes that \(|\det S| = 1\), \( S_{RL} S_{LR}^* \) is real and \(|S_{RR}| = |S_{LL}|\), or that \( T_{L \rightarrow R} \) and \( T_{R \rightarrow L} \) have the same modulus, while \( R_{L \rightarrow R} \) and \( R_{R \rightarrow L} \) have the same phase.
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• For bound states it is well known that exact PT symmetry i.e. symmetry of the Hamiltonian + symmetry of the eigenwave functions implies reality of the corresponding eigenvalues, less well known is what it means for scattering states to have
  • Asymptotic PT invariance
• To this aim, it is convenient to start from the transformation under PT of a generic wave function $\Psi(x)$
  • $PT \Psi(x) = \Psi_{PT}(x) = \Psi(-x)$
• And the condition of exact PT symmetry
  • $\Psi_{PT}(x) = \Psi(-x) = e^{i\theta} \Psi(x)$
• where $\theta$ is real, because $(PT)^2 = 1$. 
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• Let us apply the previous equation to the asymptotic wave functions
  \[ \Psi_{\text{PT}}(\pm\infty) = \Psi(-(\pm\infty)) = e^{i\theta} \Psi(\pm\infty), \]
  which implies
  \[ |T| = 1, \quad R = 0 \]
  i. e. the potential is reflectionless.

• The first example we discuss is the regularized one-dimensional form of the “centrifugal” potential
  \[ V(x) = \frac{\alpha}{(x+i\epsilon)^2} \]
  where \( \alpha \) is a real strength and \( \epsilon \) is a real constant that removes the singularity at the origin.
• The time-independent Schrödinger equation for the potential under investigation reads, in units $\hbar = 2m = 1$

$$\left( -\frac{d^2}{dx^2} + \frac{\alpha}{(x + i\epsilon)^2} \right)\Psi = k^2\Psi$$

We introduce the complex variable $z = k(x+i\epsilon)$ and express the previous equation in terms of $z$. Then, we introduce the new function $\Phi(z) = z^{1/2}\Psi(z)$. The equation satisfied by $\Phi(z)$ is a Bessel equation
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\[ z^2 \frac{d^2}{dz^2} \Phi + z \frac{d}{dz} \Phi + \left( z^2 - \alpha - \frac{1}{4} \right) \Phi = 0 \]

\begin{itemize}
  \item The square index of the Bessel equation is \( \nu^2 = \alpha + \frac{1}{4} \).
  \item A couple of linearly independent solutions to the above equation with the appropriate asymptotic behaviour for \( \Psi \) to be a scattering solution of the Schrödinger equation is provided by the Hankel functions of first and second type
\end{itemize}
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- \( \lim_{|z| \to \infty} H_\nu^{(1)}(z) = \frac{2}{(\pi z)^{1/2}} \exp[i(z-\pi \nu/2-\pi/4)] \)
- \( \lim_{|z| \to \infty} H_\nu^{(2)}(z) = \frac{2}{(\pi z)^{1/2}} \exp[-i(z-\pi \nu/2-\pi/4)] \)

valid for \( \text{Re}(\nu) > -1/2, |\text{arg } z| < \pi \).

The corresponding asymptotic solutions of the Schrödinger equation thus are

- \( \lim_{x \to \infty} \Psi_1(x) = \exp (ikx-k\epsilon -i\pi \nu/2-i\pi/4) \)
- \( \lim_{x \to \infty} \Psi_2(x) = \exp (-ikx+k\epsilon +i\pi \nu/2+i\pi/4) \)

If the above asymptotic wave functions are written as

\( \lim_{x \to \pm \infty} \Psi_m(x) = a_m e^{ikx} + b_m e^{-ikx} \)

we immediately obtain
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- \( a_{1+} = a_{1-} = \exp(-k\epsilon -i\pi \nu/2 -i\pi/4) \), \( b_{1+} = b_{1-} = 0 \),
- \( a_{2+} = a_{2-} = 0 \), \( b_{2+} = b_{2-} = \exp(k\epsilon + i\pi \nu/2 +i\pi/4) \).

- The resulting transmission and reflection coefficients are evaluated from their definitions
  - \( T_{L \rightarrow R} = (a_{2+}b_{1+} - a_{1+}b_{2+}) / (a_{2-}b_{1+} - a_{1-}b_{2+}) = 1 \),
  - \( R_{L \rightarrow R} = (b_{1+}b_{2-} - b_{1-}b_{2+}) / (a_{2-}b_{1+} - a_{1-}b_{2+}) = 0 \),
  - \( T_{R \rightarrow L} = (a_{2-}b_{1-} - a_{1-}b_{2-}) / (a_{2-}b_{1+} - a_{1-}b_{2+}) = 0 \),
  - \( R_{R \rightarrow L} = (a_{1+}a_{2-} - a_{1-}a_{2+}) / (a_{2-}b_{1+} - a_{1-}b_{2+}) = 1 \).
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• The presence of these Hankel functions suggest that it is not an accident that this potential which can be thought as obtained by some kind of dimensional reduction from the kinetic term (centrifugal barrier) in three dimensions (a kind of Kaluza-Klein dynamics in a reduced space obtained from free propagation in higher dimensions) is reflectionless.
Finally, I would like to remark that similar ideas may apply in the framework of cosmological models (Ahmed Bender Berry, Andrianov ..., t'Hooft).

The interesting remark is that by the change $x \rightarrow ix$

$$e^{-i\gamma x} \frac{\partial}{\partial x} \left( \sum_{n=0}^{\infty} a_n x^n \right) e^{i\gamma x} \frac{\partial}{\partial x} = \sum_{n=0}^{\infty} a_n \left( e^{-i\gamma x} \right)^n.$$
• one goes to a problem of wrong sign of kinetic energy and if one starts from a complex PT-symmetric potential like $ix^3$ one ends up with a real potential.

• Now this type of dynamical system is called phantom in cosmological model building.

• The discovery of the cosmic acceleration and the search for dark energy responsible for its origin have stimulated the study of field models driving the cosmological evolution. Such a study usually is called the potential reconstruction, because the most typical examples of these models are those with a scalar field, whose potential should be found to provide a given dynamics of the universe.
In the flat Friedmann models with a single scalar field, the form of the potential and the time dependence of the scalar field are uniquely determined by the evolution of the Hubble variable (up to a shift of the scalar field). Models with two scalar fields are more flexible. This is connected with the fact that experimental data may be interpreted consistently with the fact that the relation between the pressure and the energy density could be less than -1. Such equation of state arises if the matter is represented by a scalar field with a negative kinetic term. This field is called `phantom`.
Also in condensed matter physics one may wish to describe some effective particle as a negative mass particle (according to the sign of $d^2E(P)/dP^2$), then again it is useful perhaps to map this problem in a PT symmetric problem.

Non-local potentials

Let us turn now to non-local potentials: we go back to the Schrödinger equation for a wave of energy $E = k^2$

$$-(d^2/dx^2)\Psi(x) + \lambda \int K(x,y)\Psi(y)dy = k^2\Psi(x)$$

where the potential strength $\lambda$ is a real number.
In order to deal with a solvable potential, we consider only separable kernels of the kind

\[ K(x,y) = g(x)e^{i\alpha x}h(y)e^{i\beta y}, \]

where \( \alpha \) and \( \beta \) are real numbers and \( g(x) \) and \( h(y) \) are real functions of their arguments, vanishing at \( \pm \infty \).

PT invariance ( \( K(x,y) = K(-x,-y) \) ) does not impose conditions on \( \alpha \) and \( \beta \), but requires \( g(x) = g(-x) \) and \( h(y) = h(-y) \). As an important consequence, their Fourier transforms are even real functions too.

The Schrödinger equation for the problem is solved by the Green function method.
• The Green function for the problem satisfies the equation
  $$(\frac{d^2}{dx^2}) G_{\pm}(x,y) + (k^2 \pm i\varepsilon) G_{\pm}(x,y) = \delta(x-y)$$

• The infinitesimal positive number $\varepsilon$ shifts upwards, or downwards in the complex momentum plane the singularities of the Fourier transform of $G_{\pm}(x,y)$ lying on the real axis.

• The solutions are
  - $G_{+}(x,y) = -i/(2k)[ e^{ik(x-y)} \theta(x-y) + e^{-ik(x-y)} \theta(y-x) ]$
  - $G_{-}(x,y) = (G_{+}(x,y))^*$
Let us call $\Psi_\pm(x)$ two linearly independent solutions of the Schrödinger equation and define the integrals

$$I_\pm(\beta,k) = \int e^{i\beta y} h(y) \Psi_\pm(y) \, dy.$$ 

It is easy to show that $I_\pm(\beta,k)$ can be written as a convolution of the Fourier transforms of $h(y)$ and $\Psi_\pm(y)$.

The general solutions $\Psi_\pm(x)$ are implicitly written as

$$\Psi_\pm((x) = c_\pm e^{ikx} + d_\pm e^{-ikx} + \lambda I_\pm(\beta,k) \int G_\pm(x-y) g(y) e^{i\alpha y} dy$$

The above equation allows us to express $I_\pm(\beta,k)$ in terms of $c_\pm$ and $d_\pm$ as well as of Fourier transforms of known functions.
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- By multiplying both sides of the previous equation by $h(x)e^{ikx}$ and integrating over $x$ one obtains

$$I_\pm(\beta, k) = c_\pm \tilde{h}(k + \beta) + d_\pm \tilde{h}(k - \beta) + \lambda N_\pm(\alpha, \beta, k) I_\pm(\beta, k) +$$

$$N_\pm(\alpha, \beta, k) \equiv \int_{-\infty}^{+\infty} h(x)e^{i\beta x} G_\pm(x - y)g(y)e^{i\alpha y} \, dx \, dy$$
Therefore:

\[
I_{\pm}(\beta, k) = \left( c_{\pm} \tilde{h}(k + \beta) + d_{\pm} \tilde{h}(k - \beta) \right) D_{\pm}(\alpha, \beta, k)
\]

\[
D_{\pm}(\alpha, \beta, k) \equiv \frac{1}{1 - \lambda N_{\pm}(\alpha, \beta, k)}
\]
Let us examine now the asymptotic behaviour of the two independent solutions and map them to

\begin{align*}
\Psi_1(x) &\sim e^{ikx} + R_{L\rightarrow R} e^{-ikx}, & x \rightarrow -\infty \\
\Psi_1(x) &\sim T_{L\rightarrow R} e^{ikx}, & x \rightarrow +\infty \\
\Psi_2(x) &\sim T_{R\rightarrow L} e^{-ikx}, & x \rightarrow -\infty \\
\Psi_2(x) &\sim e^{-ikx} + R_{R\rightarrow L} e^{ikx}, & x \rightarrow +\infty 
\end{align*}

By a suitable choice of \( c_\pm \) and \( d_\pm \) one obtains the expressions of the transmission and reflection coefficients.
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\[ T_{L\rightarrow R} = 1 - i \omega \tilde{g}(k - \alpha) \tilde{h}(k + \beta) D_+(\alpha, \beta, k), \]
\[ R_{L\rightarrow R} = -i \omega \tilde{g}(k + \alpha) \tilde{h}(k + \beta) D_+(\alpha, \beta, k), \]
\[ T_{R\rightarrow L} = 1 - i \omega \tilde{g}(k + \alpha) \tilde{h}(k - \beta) E_- (\alpha, \beta, k), \]
\[ R_{R\rightarrow L} = -i \omega \tilde{g}(k - \alpha) \tilde{h}(k - \beta) E_- (\alpha, \beta, k). \]

- where we have put \( \omega = \lambda/(2k) \), \( D_+(\alpha, \beta, k) \) has been defined previously and the new function \( E_-(\alpha, \beta, k) \) on the right-hand-side of \( T_{R\rightarrow L} \) and \( R_{R\rightarrow L} \) is
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\[ E_-(\alpha, \beta, k) \equiv \frac{1}{1 - \lambda N_+ + i \omega \left[ \tilde{g}(k + \alpha) \tilde{h}(k - \beta) + \tilde{g}(k - \alpha) \tilde{h}(k + \beta) \right]} \]

- Detailed calculations have been performed for the one-dimensional Yamaguchi potential, where
  - \( g(x) = e^{-\gamma|x|} \), \( h(y) = e^{-\delta|y|} \),
  - with \( \gamma \) and \( \delta \) positive numbers. Defining \( \varphi(T_{a,b}) \) the phase of the complex number \( T_{a,b} \), where \( a = L \rightarrow R \), \( b = R \rightarrow L \),
  - and \( \varphi(R_{a,b}) \) the phase of \( R_{a,b} \), one obtains, for different choices of \( \alpha \) and \( \beta \), corresponding to real, hermitian, symmetric, PT-symmetric kernels
| Condition                  | $|T_a| = |T_b|$ | $\varphi(T_a) = \varphi(T_b)$ | $|R_a| = |R_b|$ | $\varphi(R_a) = \varphi(R_b)$ |
|---------------------------|-----------------|-----------------------------|-----------------|-----------------------------|
| $\alpha = \beta = 0$     | $|T_a| = |T_b|$ | $\varphi(T_a) = \varphi(T_b)$ | $|R_a| = |R_b|$ | $\varphi(R_a) = \varphi(R_b)$ |
| $\alpha = -\beta$, $\gamma = \delta$ | $|T_a| = |T_b|$ | $\varphi(T_a) \neq \varphi(T_b)$ | $|R_a| = |R_b|$ | $\varphi(R_a) = \varphi(R_b)$ |
| $\alpha = \beta \neq 0$, $\gamma = \delta$ | $|T_a| = |T_b|$ | $\varphi(T_a) = \varphi(T_b)$ | $|R_a| \neq |R_b|$ | $\varphi(R_a) = \varphi(R_b)$ |
| $\alpha \neq \beta$, $\gamma \neq \delta$ | $|T_a| = |T_b|$ | $\varphi(T_a) \neq \varphi(T_b)$ | $|R_a| \neq |R_b|$ | $\varphi(R_a) = \varphi(R_b)$ |
• **Relativistic problems**

1. Local potentials

We introduce the Dirac equation in (1+1) dimensions (units \(\hbar = c = 1\))

\[
i(\partial/\partial t)\psi(x,t) = H_D \psi(x,t) ,
\]

where the Dirac Hamiltonian with the time component of a local vector potential \(V(x) = V(-x)\) reads

\[
H_D = V(x) - i\alpha_x \partial/\partial x + \beta m .
\]

\(\alpha_x\) and \(\beta\) are 2 x 2 Dirac matrices, which we choose in the standard Dirac representation.
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\[ \alpha_x = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \beta = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

- The solution \( \psi \) to the Dirac equation in (1+1) dimensions can be written as a spinor with two components. The parity operator \( P \) and the time reversal operator \( T \) are to be defined in a consistent way. In the adopted representation, we find
  - \( P = e^{i\theta} P_0 \sigma_z \),
- where \( \theta \) is an arbitrary real constant and \( P_0 \) changes \( x \) into \( -x \).
With the above definition of $P$, it is immediate to check that $\psi_P(x,t) = P\psi(x,t)$ satisfies the Dirac equation with potential $PV(x)P^{-1} = V(-x)$.

For the time reversal operator we consistently adopt the form

\[ T = e^{i\varphi}K\sigma_z, \]

where $\varphi$ is an arbitrary real constant and $K$ performs complex conjugation. $\psi_T(x,t) = T\psi(x,t)$ satisfies the equation

\[ -i(\partial/\partial t) \psi_T(x,t) = (V(x) - i\sigma_x \partial/\partial x + m\sigma_z) \psi_T(x,t). \]

If we assume $\varphi = -\theta$, then $PT = P_0K$, like in the non-relativistic case.
We study the PT-symmetric square well potential

\[ V(x) = \begin{cases} 
  0, & x < -b \\
  V_0 - iV_1, & -b \leq x < 0 \\
  V_0 + iV_1, & 0 < x \leq +b \\
  0, & x > +b 
\end{cases} \]
In each of the four regions defined by the previous formula we search for particular solutions:

\[ \Phi(x,t) = \Phi_0(x)e^{-iEt} \]

whose spatial part can be written in the following compact form:
\( \Phi_0(x) = u_\pm(k)e^{\pm ikx} = \begin{pmatrix} u_\pm^u(k) \\ u_\pm^l(k) \end{pmatrix} e^{\pm ikx} \)

with \( k^2(x) = (E - V(x))^2 - m^2 \)

and for the ratio \( \lambda \) of lower and upper components

\[ u^l_\pm = \pm \frac{k(x)}{E - V(x) + m} u^u_\pm \equiv \pm \lambda u^u_\pm \]
The upper components, $u^\psi_z$, turn out to be arbitrary non-zero constants.

The general stationary solution, $\Psi_j(x)$, to the Dirac equation in the $J$-th region of the $x$ axis ($J = I, \ldots, IV$) can be written in the form

$$\Psi_j(x) = \begin{pmatrix} A_j e^{ik_jx} + B_j e^{-ik_jx} \\ \lambda_j (A_j e^{ik_jx} - B_j e^{-ik_jx}) \end{pmatrix},$$

where $A_j$ and $B_j$ are constant.
It is easy to express the coefficients of the general solution in region $IV \ (x \to +\infty)$ as linear functions of those in region $I \ (x \to -\infty)$. Thus we can construct two spinor wave functions $\Psi_+(x)$, representing a progressive wave ($L \to R$), and $\Psi_-(x)$, representing a regressive wave ($R \to L$), such that

$$\lim_{x \to +\infty} \Psi_+(x) = T_{L \to R} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} e^{ikx},$$

$$\lim_{x \to -\infty} \Psi_+(x) = \begin{pmatrix} 1 \\ \lambda \end{pmatrix} e^{ikx} + R_{L \to R} \begin{pmatrix} 1 \\ -\lambda \end{pmatrix} e^{-ikx},$$

$$\lim_{x \to -\infty} \Psi_-(x) = T_{R \to L} \begin{pmatrix} 1 \\ -\lambda \end{pmatrix} e^{-ikx},$$

$$\lim_{x \to +\infty} \Psi_-(x) = \begin{pmatrix} 1 \\ -\lambda \end{pmatrix} e^{-ikx} + R_{R \to L} \begin{pmatrix} 1 \\ \lambda \end{pmatrix} e^{+ikx},$$
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• The transmission and reflection coefficients in the previous formulae are expressed in terms of the $A_j$ and $B_j$ constants:

• $T_{L \rightarrow R} = A_{IV} / A_I$,

• $R_{L \rightarrow R} = B_I / A_I$,

• $T_{R \rightarrow L} = B_I / B_{IV}$,

• $R_{R \rightarrow L} = A_{IV} / B_{IV}$. 
2. Non-local potentials

The (1+1)-dimensional Dirac equation with a non-local vector-plus-scalar potential reads

\[
( -i\alpha_x \partial/\partial x + \beta m - E )\Psi(x) + ( c_S \beta + c_V ) \int dy K(x,y) \Psi(y) = 0
\]

where \( K(x,y) = g(x)e^{iax}h(y)e^{iby} \), \( a \) and \( b \) are real numbers, the real functions \( g \) and \( h \) are even functions of their argument, \( g(x) = g(-x), h(y) = h(-y) \), so as to assure PT invariance.

The solution is obtained via the Green function

\[
( -i\alpha_x \partial/\partial x + \beta m - (E \pm i\varepsilon) ) G_{\pm}(x-x') = \delta(x-x')
\]
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- whose solution is
  - \( G_\pm(x-x') = \pm i/(2k)e^{\pm k|x-x'|} \left( \pm \alpha x \text{sgn}(x-x') + \beta m + E \right). \)
- We obtain the transmission and reflection coefficients

\[
T_{L \rightarrow R} = 1 - \frac{i}{2} \tilde{g}(a-k)\tilde{h}(k+b) \frac{2}{k} \left( c_V E + c_s m \right) + i \left( c_V^2 - c_s^2 \right) \left( S_+ - D_+ \right)
\]
\[
R_{L \rightarrow R} = -\frac{i}{k} \tilde{g}(a+k)\tilde{h}(k+b) \frac{c_V m + c_s E}{1 + i \frac{S_+}{k} \left( c_V E + c_s m \right) + \frac{1}{4} \left( c_V^2 - c_s^2 \right) \left( D_+^2 - S_+^2 \right)}
\]
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where

\[ S_+(a, b, k) = N_+^{(1)}(a, b, k) + N_+^{(2)}(a, b, k) \]
\[ D_+(a, b, k) = N_+^{(1)}(a, b, k) - N_+^{(2)}(a, b, k) \]

with \( N_+^{(1)}(a, b, k) \equiv \int_{-\infty}^{+\infty} dx h(x) e^{ibx} \int_{-\infty}^{+\infty} dx' g(x') e^{i\alpha x'} e^{ik(x-x')} \theta(x-x') \)

and \( N_+^{(2)}(a, b, k) \equiv \int_{-\infty}^{+\infty} dx h(x) e^{ibx} \int_{-\infty}^{+\infty} dx' g(x') e^{i\alpha x'} e^{-ik(x-x')} \theta(x'-x) \)
Moreover

\[ T_{R \rightarrow L} = \frac{\det M_- \left( 2 \det M_- + i \tilde{g}(a - k) \tilde{h}(k + b) \left( P_{+}^{(D)} + P_{+}^{(S)} \right) \right)}{d_S} \]

\[ R_{R \rightarrow L} = \frac{i \tilde{g}(a - k) \tilde{h}(k - b) \det M_- \left( P_{+}^{(D)} - P_{+}^{(S)} \right)}{d_S} \]

where \( P_{+}^{(S)} \equiv \frac{c_{S} + c_{V}}{\lambda} - \frac{i}{2} \left( c_V^2 - c_S^2 \right) (S_- \pm D_-) \)

\[ P_{+}^{(D)} = \pm \left[ \lambda \left( c_V - c_S \right) - \frac{i}{2} \left( c_V^2 - c_S^2 \right) (S_- \pm D_-) \right] \]

\[ \det M_- = 1 - i \frac{S}{k} \left( c_V E + c_S m \right) + \frac{c_V^2 - c_S^2}{4} \left( D_-^2 - S_-^2 \right) \]
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• and

\[ d_s \equiv 2(\det M_\sim)^2 + i\g_\sim(a - k)\h_\sim(k + b) \det M_\sim \left( P_+^{(D)} + P_+^{(S)} \right) \]

\[ - i\g_\sim(a + k)\h_\sim(k - b) \det M_\sim \left( P_+^{(D)} - P_+^{(S)} \right) \]

\[ + \g_\sim(a + k)\g_\sim(a - k)\h_\sim(k + b)\h_\sim(k - b) \left( P_+^{(S)} P_+^{(D)} - P_+^{(S)} P_+^{(D)} \right) \]
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in the above formulae

\[ S_- = N_-^{(1)} + N_-^{(2)} \quad \text{and} \quad D_- = N_-^{(1)} - N_-^{(2)} \]

with

\[ N_-^{(1)}(a,b,k) = \int_{-\infty}^{+\infty} dx h(x) e^{i bx} \int_{-\infty}^{+\infty} dx' g(x') e^{ia x'} e^{-ik(x-x')} \theta(x - x') \]

and

\[ N_-^{(2)}(a,b,k) = \int_{-\infty}^{+\infty} dx h(x) e^{i bx} \int_{-\infty}^{+\infty} dx' g(x') e^{ia x'} e^{ik(x-x')} \theta(x' - x) \]
The Dirac equation satisfied by the spinor $\Psi$ reduces to two coupled equations for the spinor components $\Psi_1$ and $\Psi_2$, which decouple when $c_v = \pm c_s$.

Let us consider the case $c_v = c_s = c$ first. The two equations are

$$-\frac{d^2}{dx^2} \Psi_1(x) + 2c(m + E) \int_{-\infty}^{+\infty} dy K(x, y) \Psi_1(y) = (E^2 - m^2) \Psi_1(x) \equiv k^2 \Psi_1(x)$$

$$\Psi_2(x) = -\frac{i}{m + E} \frac{\partial}{\partial x} \Psi_1(x)$$
The previous system is suited to the study of the non-relativistic limit \( E \rightarrow m + k^2/(2m) \), with \( k^2/(2m) \ll m \): the first equation in \( \Psi_1 \) becomes a Schrödinger equation with a non-local potential of strength \( s = 2c \) and kernel \( K \).

\( \Psi_2 \), proportional to \((\partial/\partial x)\Psi_1\), does not obey a Schrödinger equation. The transmission and reflection coefficients simplify considerably:

\[
\lim_{E \rightarrow m + \frac{k^2}{2m}} T_{L \rightarrow R} = 1 - i \frac{2cm}{k} \frac{\tilde{g}(k-a)\tilde{h}(k+b)}{1 + i \frac{2cm}{k} S_+}
\]

\[
\lim_{E \rightarrow m + \frac{k^2}{2m}} R_{L \rightarrow R} = -i \frac{2cm}{k} \frac{\tilde{g}(k+a)\tilde{h}(k+b)}{1 + i \frac{2cm}{k} S_+}
\]
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• and

\[
\lim_{E \to m^+} T_{R \to L} = 1 - i \frac{2cm}{k} \frac{\tilde{g}|k + a|\tilde{h}|k - b|}{1 + i \frac{2cm}{k} \left[ - S_- + \tilde{g}|k - a|\tilde{h}|k + b| + \tilde{g}|k + a|\tilde{h}|k - b| \right]}
\]

\[
\lim_{E \to m^+} R_{R \to L} = -i \frac{2cm}{k} \frac{\tilde{g}|k - a|\tilde{h}|k - b|}{1 + i \frac{2cm}{k} \left[ - S_- + \tilde{g}|k - a|\tilde{h}|k + b| + \tilde{g}|k + a|\tilde{h}|k - b| \right]}
\]
In the case $c_v = -c_s = c'$, $\Psi_1$ and $\Psi_2$ interchange their role, since the two decoupled equations now are

$$\Psi_1(x) = -\frac{i}{E - m} \frac{\partial}{\partial x} \Psi_2(x)$$

$$- \frac{\partial^2}{\partial x^2} \Psi_2(x) + 2c'(E - m) \int_{-\infty}^{+\infty} dy K(x, y) \Psi_2(y) = \left(E^2 - m^2\right) \Psi_2(x) \equiv k^2 \Psi_2(x)$$
In the non-relativistic limit the equation for $\Psi_2$ becomes a Schrödinger equation with an energy dependent coupling strength $s(k) = c'k^2/(2m^2)$, while $\Psi_1$ is proportional to $(\partial/\partial x)\Psi_2$. The transmission and reflection coefficients now are

$$
\lim_{E \to m^+} T_{L \to R} = 1 - i \frac{c'k}{2m} \frac{\tilde{g}(k-a)\tilde{h}(k+b)}{1 + i \frac{c'k}{2m} S_+}
$$

$$
\lim_{E \to m^+} R_{L \to R} = i \frac{c'k}{2m} \frac{\tilde{g}(k+a)\tilde{h}(k+b)}{1 + i \frac{c'k}{2m} S_+}
$$
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As expected, the above formulae have the same structure as those in the case \( c_v = c_s \), with the constant strength \( s = 2c \) replaced with the energy-dependent strength \( s(k) = c'k^2/(2m^2) \).
• Conclusions

• I hope to have attracted attention on the short-range PT-symmetric potentials, which allow a discussion of scattering (continuum spectrum). For non-local separable kernels the specific choice of form factors,

• $g(x) = \exp(-c|x|)$ and $h(y) = \exp(-d|y|)$, with a cusp at the origin yields in the non-relativistic case transmission and reflection coefficients that can be written as ratios of polynomials in $k$. In the relativistic case the functional dependence is more involved due to the square root dependency on $k$ of energy $E$. 
Nevertheless, it is interesting to remark that in addition to the study of properties of $T$ and $R$ for given $c_V$ and $c_S$, one can study specific properties like absence of reflection or of transmission for a given $k$ as a function of $c_V$ and $c_S$: this can be easily done since $T$ and $R$ are, respectively, $2^{\text{nd}}$ order polynomial in $c_V$ ($c_S$) over $2^{\text{nd}}$ order polynomial and $1^{\text{st}}$ order over $2^{\text{nd}}$ order.

Analysis of the denominator of the transmission coefficient in the $-m < E < +m$ suggests that real zeros turn to complex by changing $a$ and $b$. This means that for a generic PT-symmetric kernel with a cusp at the origin one does not have a purely real spectrum.
References


10. F. Cannata, G. Junker and J. Trost, *Schrödinger operators with complex potentials but real spectrum,*
Scattering in PT-symmetric Quantum Mechanics 76


