Asymmetric scattering by non-Hermitian potentials

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Abstract – The scattering of quantum particles by non-Hermitian (generally non-local) potentials in one dimension may result in asymmetric transmission and/or reflection from left and right incidence. After extending the concept of symmetry for non-Hermitian potentials, eight generalized symmetries based on the discrete Klein’s four-group (formed by parity, time reversal, their product, and unity) are found. Together with generalized unitarity relations they determine selection rules for the possible and/or forbidden scattering asymmetries. Six basic device types are identified when the scattering coefficients (squared moduli of scattering amplitudes) adopt zero/one values, and transmission and/or reflection are asymmetric. They can pictorially be described as a one-way mirror, a one-way barrier (a Maxwell pressure demon), one-way (transmission or reflection) filters, a mirror with unidirectional transmission, and a transparent, one-way reflector. We design potentials for these devices and also demonstrate that the behavior of the scattering coefficients can be extended to a broad range of incident momenta.

Introduction. – The current interest to develop new quantum technologies is boosting applied and fundamental research on quantum phenomena and on systems with potential applications in logic circuits, metrology, communications or sensors. Robust basic devices performing elementary operations are needed to perform complex tasks when combined in a circuit.

In this paper we investigate the properties of potentials with asymmetric transmission or reflection for a quantum, spinless particle of mass \(m\) satisfying a one-dimensional (1D) Schrödinger equation. If we restrict the analysis to transmission and reflection coefficients (squared moduli of the scattering complex amplitudes) being either zero or one, a useful simplification for quantum logic operations, there are six types of asymmetric devices, see fig. 1. These devices cannot be constructed with Hermitian potentials. In fact for all device types with transmission asymmetries, which are four of the six possible devices, the potentials have to be also non-local. Therefore, non-local potentials play a major role in this paper. They appear naturally when applying partitioning techniques under similar conditions to the ones leading to non-Hermitian potentials, namely, as effective interactions for a subsystem or component of the full wave function, even if the interactions for the large system are Hermitian and local [1].

Symmetries can be used, analogously to their standard application in atomic physics to determine selection rules for allowed/forbidden transitions, to predict whether a certain potential may or may not lead to asymmetric scattering. The concept of symmetry, however, must be generalized when dealing with non-Hermitian potentials.

The theory in this paper is worked out for particles and the Schrödinger equation but it is clearly of relevance for optical devices due to the much exploited analogies and connections between Maxwell’s equations and the Schrödinger equation, which were used, e.g., to propose the realization of PT-symmetric potentials in optics [2].

Generalized symmetries. – The detailed technical and formal background for the following can be found in a previous review on 1D scattering by complex potentials [1], a companion to this article for those readers willing to reproduce the calculations in detail. The Supplemental Material (sect. I) Supplementarymaterial.pdf (SM) provides also a minimal kit of scattering theory formulae that may be read first to set basic concepts and
Table 1: Symmetries of the potential classified in terms of the commutativity or pseudohermiticity of $H$ with the elements of Klein’s 4-group \{1, II, $\Theta$, $\Pi\} \ (\text{second column}). The first column sets a simplifying roman-number code for each symmetry. The relations among potential matrix elements are given in coordinate and momentum representations in the third and fourth columns. The fifth column gives the relations they imply in the matrix elements of $S$ and/or $\bar{S}$ matrices ($S$ is for scattering by $H$ and $\bar{S}$ for scattering by $H^\dagger$). From them the next four columns set the relations implied on scattering amplitudes. Together with generalized unitarity relations (3) they also imply relations for the moduli (tenth column), and phases (not shown). The last two columns indicate the possibility to achieve perfect asymmetric transmission or reflection: “$P$” means possible (but not necessary), “No” means impossible. In some cases “$P$” is accompanied by a condition that must be satisfied.

| Code | Symmetry | (x|V|y) | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | From eq. (3) | $|T^0|=1$ | $|T^1|=1$ | $|R^0|=1$ | $|R^1|=1$ |
|------|----------|--------|----------|----------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| I    | $1H = H1$ | (x|V|y) | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| II   | $1H = H1'\Pi$ | (y|V|x)* | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | No             | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| III  | $1H = H1'\Pi$ | (y|V|x) | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | No             | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| IV   | $1H = H1'\Pi$ | (y|V|y) * | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| V    | $1H = H1\Theta$ | (y|V|x) | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| VI   | $1H = H1\Theta$ | (y|V|y) | (p|V|p') | (p|S|p') | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| VII  | $1H = H1'\Pi$ | (y|V|y) | (p|V|y) * | (p|S|y) | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |
| VIII | $1H = H1'\Pi$ | (y|V|y) | (p|V|y) | (p|S|y) | $T^0$ = $T^0$ | $T^1$ = $R^1$ | $R^1$ = $R^0$ | P              | $|T^0|=1$    | $|T^1|=1$    | $|R^0|=1$    | $|R^1|=1$    |

For a right eigenstate of $H$, $|\psi⟩$, with eigenvalue $E$, eq. (1) implies that $A|\psi⟩$ is also a right eigenstate of $H$, with the same eigenvalue if $A$ is unitary, and with the complex conjugate eigenvalue $E^*$ if $A$ is antiunitary. Equation (2) implies that $A|\psi⟩$ is a right eigenstate of $H^\dagger$ with eigenvalue $E$ for $A$ unitary or $E^*$ for $A$ antiunitary, or a left eigenstate of $H$ with eigenvalue $E^*$ for $A$ unitary, or $E$ for $A$ antiunitary. For real-energy scattering eigenfunctions in the continuum, the ones we are interested in here, $E^* = E$. When eq. (2) holds we say that $H$ is $A$-pseudo-Hermitian [4]. Parity-pseudohermiticity has played an important role as being equivalent to space-time reflection (PT) symmetry for local potentials [4,5]. A large set of these equivalences will be discussed below. A relation of the form (2) has been also used with differential operators to get real spectra beyond PT-symmetry for local potentials [6,7].

Here we consider $A$ to be a member of the Klein 4-group $K_4 = \{1, II, \Theta, II\Theta\}$ formed by unity, the parity
operator $\Pi$, the antiunitary time-reversal operator $\Theta$, and their product $\Pi \Theta$. This is a discrete, Abelian group. We also assume that the Hamiltonian is of the form $H = H_0 + V$, with $H_0$, the kinetic energy operator of the particle, being Hermitian and satisfying $[H_0, A] = 0$ for all members of the group, whereas the potential $V$ may be non-local in position representation. The motivation to use Klein’s group is that the eight relations implied by eqs. (1) and (2) generate all possible symmetries of a non-local potential due to the identity, complex conjugation, transposition, and sign inversion, both in coordinate or momentum representation, see table 1, where each symmetry has been labeled by a roman number. Interesting enough, in this classification hermiticity (symmetry II in table 1) may be regarded as 1-pseudohermiticity.

Examples how on to find the relations in the fifth column of table 1 of $S$- and $\bar{S}$-matrix elements (for scattering by $H$ and $H^\dagger$, respectively) are provided in ref. [1], where the symmetry types III, VI, and VII where worked out. Similar manipulations, making use of the action of unitary or antiunitary operators of Klein’s group on Möller operators, help to complete the table.

From the fifth column in table 1, equivalences among the amplitudes for left and right incidence for scattering by $H$, $(T^{l,r}, R^{l,r})$ or $H^\dagger (\tilde{T}^{l,r}, \tilde{R}^{l,r})$, are deduced, see the SM and the four columns for $T^{l,r}$, and $R^{l,r}$ in table 1. Together with the generalized unitarity relations $S\bar{S} = S\bar{S}^\dagger = 1$, which in terms of amplitudes take the form [1]

$$\begin{align*}
\tilde{T}^l T^l + \tilde{R}^l R^l &= 1, \\
\tilde{T}^r T^r + \tilde{R}^r R^r &= 1, \\
\tilde{T}^l R^l + \tilde{T}^r R^r &= 0, \\
T^l \tilde{R}^l + T^r \tilde{R}^r &= 0,
\end{align*}$$

these equivalences between the amplitudes imply further consequences on the amplitudes’ moduli (tenth column of table 1) and phases (not shown). The final two columns use the previous results to determine if perfect asymmetry is possible for transmission or reflection. This makes evident that hermiticity (II) and parity (III) preclude, independently, any asymmetry in the scattering coefficients; PT-symmetry (VII) or $\Theta$-pseudohermiticity (VI) forbid transmission asymmetry (all local potentials satisfy automatically symmetry VI), whereas time-reversal symmetry (i.e., a real potential in coordinate space) (V) or PT-pseudohermiticity (VIII) forbid reflection asymmetry. A caveat is that asymmetric effects forbidden by a certain symmetry in the linear (Schrödinger) regime considered in this paper might not be forbidden in a non-linear regime [8], which goes beyond our present scope.

The occurrence of one particular symmetry in the potential (conventionally “first symmetry”) does not exclude a second symmetry to be satisfied as well. When a double symmetry holds, excluding the identity, the “first” symmetry implies the equivalence of the second symmetry with a third symmetry. We have already mentioned that II-pseudohermiticity (IV) is equivalent to PT-symmetry (VII) for local potentials. Being local is just one particular way to satisfy symmetry VI, namely $\Theta$-pseudohermiticity. The reader may verify with the aid of the third column for $\langle x|V|y \rangle$ in table 1, that indeed, if symmetry VI is satisfied (first symmetry), symmetry IV has the same effect as symmetry VII. They become equivalent. Another well-known example is that for a local potential (symmetry VI is satisfied), a real potential in coordinate space is necessarily Hermitian, so symmetries V and II become equivalent. These examples are just particular cases of the full set of equivalences given in table 2.

Combining the information of the last two columns in table 1 with the additional condition that all scattering coefficients be 0 or 1 we elaborate table 3, which provides the symmetries that do not allow the implementation of the devices in fig. 1. The complementary table 4 gives instead the symmetries that allow, but do not necessarily imply, a given device type. The device denominations in fig. 1 or table 3 are intended as short and meaningful, and do not necessarily coincide with some extended terminology, in part because the range of possibilities is broader here than those customarily considered, and because we use a 1 or 0 condition for the moduli. For example, a device with reflection asymmetry and with $T^r = T^l = 1$ would in our case be a particular “transparent, one-way reflector”, as full transmission occurs from both sides. This effect has however become popularized as “unidirectional invisibility” [9,10]. A debate on terminology is not our main concern here, and the use of a code system as the one proposed will be instrumental in avoiding misunderstandings.

**Designing potentials for asymmetric devices.** – We will show how to design non-local potentials leading
to the asymmetric devices. For simplicity we look for non-local potentials \( V(x,y) \) with local support that vanish for \( |x| > d \) and \( |y| > d \).

Inverse scattering proceeds similarly to [12], by imposing an ansatz for the wave functions and the potential in the stationary Schrödinger equation

\[
\frac{\hbar^2 k^2}{2m} \psi(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \int_{-d}^{d} dy V(x,y) \psi(y). \tag{4}
\]

The free parameters are fixed making use of the boundary conditions. The form of the wave function incident from the left is \( \psi_l(x) = e^{ikx} + R_l e^{-ikx} \) for \( x < -d \) and \( \psi_l(x) = T_i e^{ikx} \) for \( x > d \), where \( k = p/\hbar \). The wave function incident from the right is instead \( \psi_r(x) = e^{-ikx} T_r \) for \( x < -d \) and \( \psi_r(x) = e^{-ikx} + R_r e^{ikx} \) for \( x > d \).

Our strategy is to assume polynomial forms for the two wave functions in the interval \( |x| < d \), \( \psi_l(x) = \sum_{j=0}^{5} c_{l,j} x^j \) and \( \psi_r(x) = \sum_{j=0}^{5} c_{r,j} x^j \), and also a polynomial ansatz of finite degree for the potential \( V(x,y) = \sum_{j=0}^{5} \sum_{y=0}^{5} v_{j,y} x^j y^j \). Inserting these ansatzes in eq. (4) and from the conditions that \( \psi_{l,r} \) and their derivatives must be continuous, all coefficients \( c_{l,j} \), \( c_{r,j} \) and \( v_{j,y} \) can be determined. Symmetry properties of the potential can also be imposed via additional conditions on the potential coefficients \( v_{j,y} \). For example we may use this method to obtain a one-way T-filter \( (T/A) \) device (third device in table 3) with a non-local PT-pseudo-Hermitian potential (symmetry VIII of table 1) for a chosen wave vector \( k = k_0 \). The absolute value and argument of the resulting potential \( V(x,y) \) are shown in figs. 2(a) and (b) together with its scattering coefficients as function of the incident wave vector, fig. 2(c). As can be seen in fig. 2(c) the imposed scattering coefficients are fulfilled exactly for the chosen wavevector. They are also satisfied approximately in a neighborhood of \( k_0 \). In the SM (sect. II) we give further details about the construction of this potential and we work out other asymmetric devices of fig. 1.

### Extending the scattering asymmetry to a broad incident-momentum domain.

The inversion technique just described may be generalized to extend the range of incident momenta for which the potential works by imposing additional conditions and increasing correspondingly the number of parameters in the wavefunction ansatz, for example we may impose that the derivatives of the amplitudes, in one or more orders, vanish at \( k_0 \), or \( 0/1 \) values for the coefficients not only at \( k_0 \) but at a series of grid points \( k_1 \), \( k_2 \), ..., \( k_N \), as in [11,12–14].

Here we put forward instead a method that provides a very broad working-window domain. While we make formally use of the Born approximation, the exact numerical computations demonstrate the robustness and accuracy of the approach to achieve that objective by making use of an adjustable parameter in the potential. The very special role of the Born approximation in inverse problems has been discussed and demonstrated in [15–17]. Specifically we study a transparent one-way reflector \( T/R/T \).

Our aim is now to find a local PT-symmetric potential such that asymmetric reflection results, \( T^i = T^r = 1, R^i = 0, |R^r| = 1 \) for a broad range of incident momenta. A similar goal was pursued in [18] making use of a supersymmetric transformation, without imposing \( |R^r| = 1 \).

In the Born approximation and for a local potential \( V(x) \), the reflection amplitudes take the simple form

\[
R^i = -\frac{2\pi im}{p} (-p|V|p), \quad R^r = -\frac{2\pi im}{p} (p|V| - p). \tag{5}
\]

Defining the Fourier transform

\[
\hat{V}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \hspace{1em} V(x) e^{-ikx}, \tag{6}
\]

we get for \( k = p/\hbar > 0 \)

\[
R^i = -\frac{\sqrt{2\pi im}}{kh^2} \hat{V}(-2k), \quad R^r = -\frac{\sqrt{2\pi im}}{kh^2} \hat{V}(2k). \tag{7}
\]
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Assuming that the potential is local and PT-symmetrical, we calculate the transition coefficient from them using generalized unitarity as $|T|^2 = 1 - R^* R^\dagger$.

To build a $TR/T$ device we demand: $\hat{V}(k) = \sqrt{2\alpha}k \epsilon (k < 0)$ and $\hat{V}(k) = 0 (k \geq 0)$. By inverse Fourier transformation, this implies

$$ V(x) = -\alpha \frac{\partial}{\partial x} \lim_{\epsilon \to 0} \frac{1}{(x - i \epsilon)^2} = \alpha \int_{-\infty}^{\infty} (x^2 - \epsilon^2)^2 + \frac{2x \epsilon}{(x^2 + \epsilon^2)^2} \, dx, $$

which is indeed a local, PT-symmetric potential for $\alpha$ real. $\alpha$ is directly related to the reflection coefficient, within the Born approximation, $R^\dagger = 4\pi \text{Im} / \hbar^2$. As the Born approximation may differ from exact results we shall keep $\alpha$ as an adjustable parameter in the following.

In a possible physical implementation, the potential in eq. (8) will be approximated by keeping a small finite $\epsilon > 0$, see fig. 3(a). Then, its Fourier transform is $\hat{V}(k) = \sqrt{2\alpha} \epsilon e^{ik \epsilon} (k < 0)$ and $\hat{V}(k) = 0 (k \geq 0)$. In figs. 3(b) and (c), the resulting coefficients for $\epsilon/d = 10^{-4}$ and two different values of $\alpha$ are shown. These figures have been calculated by numerically solving the Schrödinger equation exactly. Remarkably, the Born approximation contains all the information required to build the required potential shape up to a global factor. Such a prominent role of the Born approximation in inverse problems has been noted in different applications [15–17]. For a range of $\alpha$, the potential gives $|R|^2 \approx 0$, a nearly constant $|R^\dagger|^2$, and $|T^\dagger| = |T|^\dagger \approx 1$ in a broad $k$-domain, see fig. 3(b). Adjusting the value of $\alpha$, fig. 3(c), sets $|R|^2 \approx 1$ as desired.

**Discussion.** – Scattering asymmetries are necessary to develop technologically relevant devices such as one-way mirrors, filters and barriers, invisibility cloaks, diodes, or Maxwell demons. So far much effort has been devoted to build and apply local PT-symmetric potentials but the possible scattering asymmetries with them are quite limited. We find that six device types with asymmetric scattering are possible when imposing 0 or 1 scattering coefficients. PT-symmetry can only realize one of them, but this symmetry is just one among eight possible symmetries of complex non-local potentials. The eight symmetries arise from the discovery that Klein’s four-group $\{1, \Pi, \Theta, \Theta\Pi\}$, combined with two possible

Fig. 2: (Color online) One-way T-filter ($T/A$, $|T|^2 = 1, T^\dagger = R^\dagger = R^\epsilon = 0$) with potential $V(x, y) = |V(x, y)| e^{i\phi(x, y)}$ set for $k_0 = 1/d$. (a) Absolute value $|V(x, y)|$; (b) argument $\phi(x, y)$; (c) transmission and reflection coefficients: $|R^2|$ (black, solid line), $|R^\dagger|^2$ (green, solid line), $|R^\epsilon|^2$ (blue, thick, dashed line), $|T^\dagger|^2$ (red, dotted line). $V_0 = \hbar^2/(2md^2)$.

Fig. 3: (Color online) Transparent 1-way reflector with a local PT potential: (a) approximation of the potential (8), real part (green solid line), imaginary part (blue dashed line). (b), (c) Transmission and reflection coefficients vs. momentum $kd$; left incidence: $|R^\epsilon|^2$ (black, solid line), $|T^\dagger|^2$ (green, solid line); right incidence: $|R^\epsilon|^2$ (blue, thick, dashed line), $|T^\dagger|^2$ (red, dotted line, coincides with green, solid line). $\epsilon/d = 10^{-4}$. (b) $\alpha = 1.0k^2/(4\pi m)$ (c) $\alpha = 1.25k^2/(4\pi m)$ (the black, solid line coincides here mostly with the red, dotted and green, solid lines).

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relations among the Hamiltonian, its adjoint, and the symmetry operators of the group, eqs. (1) and (2), produce all possible equalities among potential matrix elements after complex conjugation, coordinate inversion, the identity, and transposition. In other words, to have all possible such equalities, the conventional definition of a symmetry $A$ in terms of its commutation with the Hamiltonian $H$ is not enough, and $A$-pseudohermiticity must be considered as well on the same footing. Extending the concept of what a symmetry is for complex, non-local potentials is a fundamental, far-reaching step of this work. This group theoretical analysis and classification is not only esthetically pleasing, but also of practical importance, as it reveals the underlying structure and span of the possibilities available in principle to manipulate the asymmetrical response of a potential for a structureless particle.

We provide potentials for the different asymmetric devices including an example that works in a broad domain of incident momenta. Although the present theory is for the scattering of quantum particles, the analogues between quantum physics and optics suggest to extend the concepts and results for optical asymmetric devices.

Interesting questions left for future work are the inclusion of other mechanisms for transmission and reflection asymmetries (for example non-linearities [8,19], and time-dependent potentials [20,21]), or a full discussion of the phases of the scattering amplitudes in addition to the moduli emphasized here. In this paper the properties of the scattering amplitudes have been worked out assuming that the operator $A$ in the symmetry relations in eqs. (1) and (2) is a unitary/antiunitary operator in Klein’s group. We may generalize the study to include more general operators, possibly including differential operators, as was done in [22] for phase transitions of optical potentials, or the operator that swaps internal states or waveguides [23,24].

We shall also examine in a complementary paper the physical realization of complex non-local effective potentials. In a quantum optics scenario, simple examples were provided in [25] based on applying the partitioning technique [26,27] to the scattering of a particle with internal structure. The experimental realization of all new symmetries and devices may be challenging, e.g., to engineer the non-locality in optics, but there is much to gain. We may expect progress similar to the successful evolution from theory to actual devices in the sequence from the first mathematical models of PT-symmetric potentials [28], to the proposal of an optical realization [2], and to the actual experiments [29], even if considerable time lapsed were needed between the three steps.

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