S-matrix pole symmetries for non-Hermitian scattering Hamiltonians

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The complex eigenvalues of some non-Hermitian Hamiltonians, e.g., parity-time-symmetric Hamiltonians, come in complex-conjugate pairs. We show that for non-Hermitian scattering Hamiltonians (of a structureless particle in one dimension) possessing one of four certain symmetries, the poles of the S-matrix eigenvalues in the complex momentum plane are symmetric about the imaginary axis, i.e., they are complex-conjugate pairs on the complex-energy plane. This applies even to states which are not bounded eigenstates of the system, i.e., antibound or virtual states, resonances, and antiresonances. The four Hamiltonian symmetries are formulated as the commutation of the Hamiltonian with specific antilinear operators. Example potentials with such symmetries are constructed and their pole structures and scattering properties are calculated.

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I. INTRODUCTION

Non-Hermitian (NH) Hamiltonians may represent effective interactions for components of a system. Feshbach's partitioning technique [1,2] provides the formal framework to find NH Hamiltonians for a subspace from the Hermitian Hamiltonian for the total system. NH Hamiltonians are also set phenomenologically to mimic some observed or desired behavior, such as gain, decay, or absorption in nuclear or atomic, molecular, and optical physics [3–8]. They arise as well as auxiliary tools to facilitate calculations of cross sections or resonances, e.g., by complex scaling of the coordinates [9,10], and also to model some open systems [11] and lattices [12].

Much work on NH physics has focused on parity-time (PT)–symmetric Hamiltonians, as they may have a purely real spectrum [13]. More recently, other NH and non-PT Hamiltonians have been shown to hold real eigenvalues [14–16]. Work on scattering by PT-symmetric potentials was at first rather scarce [3,17–19]. However, scattering has been later investigated intensely in connection with spectral singularities and reflection asymmetries for left or right incidence (i.e., unidirectional invisibility) [20–22], in most cases restricting the analysis to local potentials. Interestingly, it has been recently shown that different devices with asymmetrical scattering responses [i.e., with different transmission and/or reflection for right and left incidence in a one-dimensional (1D) setting] are possible if one makes use of nonlocal potentials [23]. Reference [23] provides the selection rules for the transmission and reflection coefficient asymmetries based on eight basic Hamiltonian symmetries. Four of these symmetries are of the standard form,

$$AH = HA, \tag{1}$$

and the other four are of the form

$$AH = H^{\dagger}A, \tag{2}$$

where A is a unitary or antiunitary operator in Klein's 4-group $\mathbf{K}_4 = \{1, \Pi, \Theta, \Theta\Pi\}$ formed by the identity (1), parity (Π), time reversal (Θ), and their product ($\Theta\Pi$), also termed PT. A Hamiltonian which has symmetry (2) is called A-pseudo-Hermitian.

Here we aim at extending further our understanding of scattering of a structureless particle by NH potentials in one dimension by considering general potentials that are not necessarily diagonal in coordinate representation (i.e., nonlocal potentials). These typically arise when applying Feshbach's partitioning technique [24]. The results of [23] are expanded in several directions:

(i) We provide an alternative characterization of the above-mentioned eight symmetries in terms of the invariance of H with respect to the action of superoperators. We also show that the four symmetries associated with A-pseudohermiticity relations, (2), can be formulated as well as the commutativity of H with certain operators (linear if A is antilinear and antilinear if A is linear). This formulation extends earlier results for Hamiltonians with a discrete spectrum [25,26].

(ii) Moreover, four of these eight symmetries imply the same type of pole structure of S-matrix eigenvalues in the complex momentum plane that was found for PT symmetry [3], namely, zero-pole correspondence at complex-conjugate points and poles on the imaginary axis or forming symmetrical pairs with respect to the imaginary axis [27]. This configuration with poles located on the imaginary axis or as symmetrical pairs has some important consequences. In particular, it provides stability of the real energy eigenvalues with respect to parameter variations of the potential. While a simple pole on the imaginary axis can move along that axis when a parameter is changed, it cannot move off this axis (since this would violate the pole-pair symmetry) or bifurcate.

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The formation of pole pairs occurs near special parameter values for which two poles on the imaginary axis collide.

The remainder of the article is organized as follows. In Sec. II we review the scattering properties of eight different Hamiltonian symmetries. These symmetries may be characterized as commutativity or pseudohermiticity with respect to four unitary or antiunitary operators forming a Klein 4-group or as invariance with respect to the action of eight linear or antilinear superoperators. In Sec. III we discuss the physical consequences of the symmetries in the pole structure of the scattering matrix eigenvalues and hence in the transmission and reflection amplitudes. Four symmetries are shown to lead to complex poles corresponding to real energies or conjugate (energy) pairs. In Sec. IV we exemplify the general results with separable potentials exhibiting parity pseudohermiticity and time-reversal symmetry. These are the two nontrivial symmetries of the four (in the sense that the other two, hermiticity and PT symmetry, have already been well discussed). In Sec. V we discuss and summarize our results.

II. HAMILTONIAN SYMMETRIES

A. Basic concepts and terminology

Let us first clarify the terminology. Scattering Hamiltonians are those that can be written as the sum of the kinetic energy $H_0 = p^2/(2m)$ operator and a potential energy operator V,

$$H = H_0 + V. \tag{3}$$

V is in general nonlocal, i.e., it does not have the local form $\langle x|V|x'\rangle = \delta(x - x')V(x)$. Apart from their generic appearance in Feschbach's partitioning technique (see, e.g., [24]), nonlocal potentials are quite common in models that discretize the coordinates at specific sites, as in tight-binding models. These are widely used for describing condensed matter and ultracold atoms in a lattice. For example, the well-known Bose-Hubbard model has been generalized to a non-Hermitian Hamiltonian to account for dissipation effects (see, e.g., [28] and [29]). However, here we limit ourselves to continuous-coordinate scattering models [30]. The potential function in position coordinates $V(x, x') = \langle x|V|x'\rangle$ is assumed to decay rapidly enough to 0 when a position goes to ∞ so that the usual operators of scattering theory are well defined and the Hilbert space is (biorthogonally) decomposed into a continuum part with real eigenvalues and a discrete part. See Appendix A for a review of the formalism and notation we use.

We now discuss the eight symmetries identified in [23], which are associated with the two generalized symmetry relations corresponding to commutation with A and A-pseudohermiticity [25]; see Eqs. (1) and (2). We use Roman numerals to label these symmetries as reported in Table I: I ($1H = H1$, the trivial identity); II ($1H = H^\dagger 1$, hermiticity or "1-pseudohermiticity"); III ($\Pi H = H\Pi$, parity); IV ($\Pi H = H^\dagger\Pi$, Π-pseudohermiticity); V ($\Theta H = H\Theta$, time-reversal invariance); VI ($\Theta H = H^\dagger\Theta$, Θ-pseudohermiticity); VII ($\Pi\Theta H = H\Pi\Theta$, PT symmetry); and VIII ($\Pi\Theta H = H^\dagger\Theta\Pi$, $\Pi\Theta$-pseudohermiticity). Note that a local potential would automatically fulfill symmetry VI but this symmetry does not necessarily imply locality. For local potentials four of the eight symmetries coincide with the other four [23]. Here we consider general nonlocal potentials where all the eight symmetries are distinct.

The generalization of the symmetry concept to the pair (1) and (2) is in fact quite natural if we take into account that an NH H has generically different left and right eigenvectors. Given a right eigenstate $|\psi\rangle$ of H with eigenvalue E, Eq. (1) implies that $A|\psi\rangle$ is also a right eigenvector with eigenvalue E or E^*, whereas Eq. (2) implies that $\langle\psi|A$ is a left eigenvector of H with eigenvalue E^* or E, for A unitary or antiunitary, respectively [31]. The symmetries which imply the presence of real or complex-conjugate pairs of energy eigenvalues for bound eigenstates are II, IV, V, and VII. The emergence of these complex-conjugate pairs has been discussed in [25] and [32] for a general class of diagonalizable Hamiltonians that possess a discrete spectrum. They can be heuristically understood for the symmetries we consider as follows: Symmetry V implies that the Hamiltonian must be real in coordinate space, which would lead to a real characteristic polynomial with real or complex-conjugate roots. Symmetry VII is PT symmetry, which is well discussed in the literature as having real or complex-conjugate pairs of eigenvalues [13]. Note

TABLE I. Symmetries of the potential based on the commutativity or pseudohermiticity of H with the elements of $\mathbf{K}_4$ (column 2). Columns 3, 5, and 7 to 11 are to be read as follows: For each symmetry the object in the column is equal to the one in the top row of the column. The relations among potential matrix elements are given in coordinate and momentum representations in columns 3 and 5. In columns 4 and 6, each symmetry is regarded as the invariance of the potential with respect to the transformations represented by superoperators $\mathcal{L}$ (see Sec. II B) in coordinate or momentum representation. Column 5 gives the relations they imply in the matrix elements of S and $\widehat{S}$ matrices. Columns 8–11 set the relations for the scattering amplitudes.

(1) Code	(2) Symmetry	(3) $\langle x\|V\|y\rangle$	(4) $\mathcal{L}$(coord)	(5) $\langle p\|V\|p'\rangle$	(6) $\mathcal{L}$(momentum)	(7) $\langle p\|S\|p'\rangle$	(8) T^l	(9) T^r	(10) R^l	(11) R^r
I	$1H = H1$	$\langle x\|V\|y\rangle$	1	$\langle p\|V\|p'\rangle$	1	$\langle p\|S\|p'\rangle$	T^l	T^r	R^l	R^r
II	$1H = H^\dagger 1$	$\langle y\|V\|x\rangle^*$	$\mathcal{T}\mathcal{C}$	$\langle p'\|V\|p\rangle^*$	$\mathcal{T}'\mathcal{C}'$	$\langle p\|\widehat{S}\|p'\rangle$	$\widehat{T}^l$	$\widehat{T}^r$	$\widehat{R}^l$	$\widehat{R}^r$
III	$\Pi H = H\Pi$	$\langle -x\|V\|-y\rangle$	$\mathcal{I}$	$\langle -p\|V\|-p'\rangle$	$\mathcal{I}'$	$\langle -p\|S\|-p'\rangle$	T^r	T^l	R^r	R^l
IV	$\Pi H = H^\dagger\Pi$	$\langle -y\|V\|-x\rangle^*$	$\mathcal{C}\mathcal{T}I$	$\langle -p'\|V\|-p\rangle^*$	$\mathcal{C}'\mathcal{T}'I'$	$\langle -p\|\widehat{S}\|-p'\rangle$	$\widehat{T}^r$	$\widehat{T}^l$	$\widehat{R}^r$	$\widehat{R}^l$
V	$\Theta H = H\Theta$	$\langle x\|V\|y\rangle^*$	$\mathcal{C}$	$\langle -p\|V\|-p'\rangle^*$	$\mathcal{I}'\mathcal{C}'$	$\langle -p'\|\widehat{S}\|-p\rangle$	$\widehat{T}^r$	$\widehat{T}^l$	$\widehat{R}^l$	$\widehat{R}^r$
VI	$\Theta H = H^\dagger\Theta$	$\langle y\|V\|x\rangle$	$\mathcal{T}$	$\langle -p'\|V\|-p\rangle$	$\mathcal{I}'\mathcal{T}'$	$\langle -p'\|S\|-p\rangle$	T^r	T^l	R^l	R^r
VII	$\Theta\Pi H = H\Theta\Pi$	$\langle -x\|V\|-y\rangle^*$	$\mathcal{I}\mathcal{C}$	$\langle p\|V\|p'\rangle^*$	$\mathcal{C}'$	$\langle p'\|\widehat{S}\|p\rangle$	$\widehat{T}^l$	$\widehat{T}^r$	$\widehat{R}^r$	$\widehat{R}^l$
VIII	$\Theta\Pi H = H^\dagger\Theta\Pi$	$\langle -y\|V\|-x\rangle$	$\mathcal{I}\mathcal{T}$	$\langle p'\|V\|p\rangle$	$\mathcal{T}'$	$\langle p'\|S\|p\rangle$	T^l	T^r	R^r	R^l

also that the matrix elements of PT-symmetric Hamiltonians are real in the momentum representation. More generally, in [26], it was shown, for diagonalizable Hamiltonians having a discrete spectrum, that A-pseudohermiticity for a Hermitian invertible linear operator A is equivalent to the presence of an ordinary symmetry of the form $BH = HB$ for some antilinear operator B with $B^2 = 1$. Because B is an antilinear operator, the eigenvectors $|E_n\rangle$ of H with eigenvalues E_n satisfy

$$HB|E_n\rangle = BH|E_n\rangle = E_n^* B|E_n\rangle. \tag{4}$$

Therefore complex eigenvalues E_n come in complex-conjugate pairs. In particular, when $|E_n\rangle$ is an eigenvector of B, i.e., $B|E_n\rangle = e^{ib_n}|E_n\rangle$ for some real number b_n, we have $E_n \in \mathbb{R}$. The proof of the equivalence of A-pseudohermiticity for linear A and the presence of ordinary antilinear symmetries given in [26] relies on the observation that every diagonalizable Hamiltonian with a discrete spectrum is τ-pseudo-Hermitian for some invertible Hermitian antilinear operator τ, i.e., $\tau H = H^\dagger \tau$. This relation together with Eq. (2) implies $BH = HB$, if we set $B = A^{-1}\tau$. (If $AH = H^\dagger A$ and A is a Hermitian antilinear operator, a linear $B = A^{-1}\tau$ can also be constructed so that $BH = HB$, but the E_n do not form conjugate pairs.) In Appendix B we extend this construction to scattering potentials.

In summary, the symmetries with conjugate pairs II, IV, V, and VII can all be expressed as the commutation of H with a certain antilinear operator, as seen directly in the symmetries V and VII, in which H commutes with an antilinear A, and by constructing an antilinear B in symmetries II and IV. An aspect uncovered in this paper is that whenever one of the above-mentioned four symmetries holds, not only do the complex eigenvalues representing the bound states come in conjugate-complex pairs, but all the complex poles of the S matrix have this property.

B. Superoperator formalism

The eight symmetries listed in Table I may also be regarded as the invariance of the Hamiltonian matrix with respect to transformations represented by superoperators $\mathcal{L}$ [33] defined by

$$\mathcal{L}(H) = \begin{cases} A^\dagger H A: & \text{I, III,V, VII} \\ A^\dagger H^\dagger A: & \text{II, IV, VI, VIII} \end{cases} \tag{5}$$

This definition of the superoperator action is independent of the representation we use, but its realization in coordinates or momenta in terms of the operations of complex conjugation, transposition, and inversion is different. For example, in coordinate representation, these three operations and unity take the following superoperator forms (see column 3 in Table I),

$$\begin{aligned} 1H &= \iint |x\rangle\langle x|H|y\rangle\langle y|dxdy, \\ \mathcal{T}(H) &= \iint |x\rangle\langle y|H|x\rangle\langle y|dxdy, \\ \mathcal{C}(H) &= \iint |x\rangle\langle x|H|y\rangle^*\langle y|dxdy, \\ \mathcal{I}(H) &= \iint |x\rangle\langle -x|H|-y\rangle\langle y|dxdy. \end{aligned} \tag{6}$$

Adopting the following inner product for linear operators F and G, $\langle\langle F|G\rangle\rangle = \mathrm{tr}F^\dagger G$, we can show that all superoperators $\mathcal{L}$ are either unitary (for $\mathcal{L} = 1, \mathcal{T}, \mathcal{I}, \mathcal{TI}$) or antiunitary (for $\mathcal{L} = \mathcal{C}, \mathcal{CT}, \mathcal{CI}, \mathcal{CTI}$), as defined by

$$\langle\langle \mathcal{L}F|\mathcal{L}G\rangle\rangle = \langle\langle F|G\rangle\rangle \quad (\mathcal{L}\text{ unitary}), \tag{7}$$

$$\langle\langle \mathcal{L}F|\mathcal{L}G\rangle\rangle = \langle\langle F|G\rangle\rangle^* \quad (\mathcal{L}\text{ antiunitary}). \tag{8}$$

They all satisfy $\mathcal{L}\mathcal{L}^\dagger = \mathcal{L}^\dagger\mathcal{L} = 1$, where the adjoints are defined differently for linear or antilinear superoperators:

$$\langle\langle F|\mathcal{L}^\dagger G\rangle\rangle = \langle\langle \mathcal{L}F|G\rangle\rangle \quad (\mathcal{L}\text{ unitary}), \tag{9}$$

$$\langle\langle F|\mathcal{L}^\dagger G\rangle\rangle = \langle\langle \mathcal{L}F|G\rangle\rangle^* \quad (\mathcal{L}\text{ antiunitary}). \tag{10}$$

Moreover, the eight superoperators satisfy $\mathcal{L}^\dagger = \mathcal{L}$.

The set $\{1, \mathcal{I}, \mathcal{T}, \mathcal{C}, \mathcal{CT}, \mathcal{TI}, \mathcal{IC}, \mathcal{CTI}\}$ forms the elementary abelian group $E8$ [34]. This is a homocyclic group, namely, the direct product of isomorphic cyclic groups of order 2 with generators $\mathcal{C}, \mathcal{T}, \mathcal{I}$. We may, similarly to Eq. (6), define primed superoperators in momentum representation, e.g., $\mathcal{T}'H = \iint |p\rangle\langle p'|H|p\rangle\langle p'|dp\,dp'$. They also form the E8 group $\{1, \mathcal{I}', \mathcal{T}', \mathcal{C}', \mathcal{C}'\mathcal{T}', \mathcal{T}'\mathcal{I}', \mathcal{I}'\mathcal{C}', \mathcal{C}'\mathcal{T}'\mathcal{I}'\}$. Only for the subgroup $\{1, \mathcal{I}, \mathcal{CT}, \mathcal{CTI}\}$ do the superoperators have the same representation-independent form in terms of complex conjugation, transposition, and inversion.

A direct application of the superoperator framework is the generalization of Wigner's formulation of symmetries [35]. He associated symmetry transformations with unitary or antiunitary operators preserving the (Hilbert-space) inner product, namely, the "transition probabilities" $|\langle A\psi, A\phi\rangle|^2 = |\langle\psi, \phi\rangle|^2$. For general states described by density operators ρ_1, ρ_2, transition probabilities are computed as $\langle\langle\rho_1|\rho_2\rangle\rangle$ and the transformations described by the unitary or antiunitary superoperators preserve the transition probability. Hamiltonian symmetries are, within the conventional Wigner scheme, the symmetry transformations that leave the Hamiltonian invariant ($A^\dagger H A = H$, so that A and H commute). Here the Hamiltonian symmetry is more broadly defined as the invariance $\mathcal{L}H = H$, which includes transformations beyond the conventional scheme.

III. S-MATRIX POLE STRUCTURE

To derive the results in [23] extensive use of the scattering matrix (S-matrix) formalism was made. The full S-matrix provides outgoing waves when acting on incoming waves. It is typically decomposed into on-the-energy-shell matrices. In 1D scattering, the on-the-energy-shell S matrix for H is defined on the real positive momentum axis in terms of transmission and reflection amplitudes for right and left incidence [3],

$$\mathsf{S} = \begin{pmatrix} T^l(p) & R^r(p) \\ R^l(p) & T^r(p) \end{pmatrix}. \tag{11}$$

There is a companion matrix $\widehat{\mathsf{S}}$ with hatted amplitudes corresponding to scattering by $H^\dagger$. See Appendix A and [3] for details. The S matrix contains the scattering amplitudes for incoming wave packets with well-defined momenta being scattered into states with the same kinetic energy and reflected and transmitted components. For negative p the matrix elements give the amplitudes of scattering states with a pure outgoing plane wave towards the right or the left. Moreover, we assume, as is customary, that the amplitudes may be continued analytically beyond the real axis. The existence of a continuation on a complex plane domain depends on the decay properties of the potentials and may be checked for each potential. The analytical continuation is indeed possible for the model potentials of the following section.

The eigenvalues of S can be calculated from the transmission and reflection amplitudes as

$$S_j = \frac{(T^l + T^r) + (-1)^j[(T^l - T^r)^2 + 4R^lR^r]^{1/2}}{2} \tag{12}$$

for $j = 1, 2$, and of course there is a similar expression for $\widehat{S}_j$ with hatted amplitudes. In general they satisfy the relations [3]

$$S_j(p) = \widehat{S}^*_j(-p^*) \tag{13}$$

and

$$\widehat{S}^*_j(p^*)S_j(p) = 1\,. \tag{14}$$

Combining Eqs. (13) and (14) gives

$$S_j(p) = S_j^{-1}(-p)\,. \tag{15}$$

Equation (15) is remarkable since it reveals the presence of a pole (zero) at $-p$ if there is a zero (pole) at p. If the following relations are fulfilled,

$$T^{r,l}(p) = \widehat{T}^{r,l}(p) \quad \text{or} \quad T^{r,l}(p) = \widehat{T}^{l,r}(p), \tag{16}$$

$$R^{r,l}(p) = \widehat{R}^{r,l}(p) \quad \text{or} \quad R^{r,l}(p) = \widehat{R}^{l,r}(p), \tag{17}$$

then

$$S_j(p) = \widehat{S}_j(p), \tag{18}$$

which, together with Eq. (13), gives

$$S_j(p) = S^*_j(-p^*). \tag{19}$$

In plain language, Eq. (19) tells that if Eqs. (16) and (17) are satisfied, the poles and zeros of S_j must be symmetrically distributed with respect to the imaginary axis of the momentum complex plane. Combined with Eq. (15) this also means that each pole has a symmetrical zero with respect to the real axis. This symmetrical distribution of poles and zeros is the same as in the Hermitian case (see Fig. 1), the only difference being the possibility of finding pairs of symmetrical poles in the upper complex plane when $H \neq H^\dagger$. They represent normalizable "bound states with complex energies." When they are not present, the discrete spectrum becomes purely real.

According to Table I, Eqs. (16) and (17) are fulfilled for symmetries II (hermiticity), VII (PT symmetry), IV (parity pseudohermiticity), and V (time-reversal invariance). Thus, Hamiltonians having these symmetries have their S-matrix poles symmetrically distributed around the imaginary axis. For local potentials the last two symmetries coalesce with the first two well-known cases [23], namely, IV becomes equivalent to PT symmetry, and V becomes equivalent to hermiticity. For nonlocal potentials, though, these symmetries

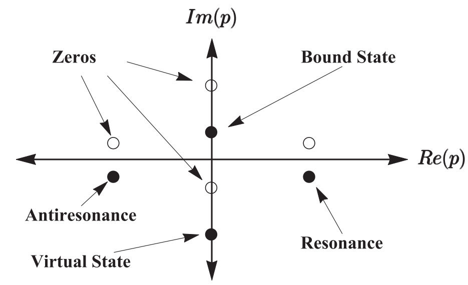

FIG. 1. Example of configuration of poles (filled circles) and zeros (open circles) of the S-matrix eigenvalues in the complex momentum plane for Hermitian Hamiltonians. Poles in the upper half-plane [Im(p) > 0] correspond to bound eigenstates of the Hamiltonian, i.e., localized states with negative energy. Poles in the lower half-plane correspond to virtual states [Re(p) = 0], resonances [Re(p) > 0], and antiresonances [Re(p) < 0]. Singularities with a negative imaginary part correspond to states that do not belong to the Hilbert space since they are not normalizable. However, they can produce observable effects in the scattering amplitudes, in particular, when they approach the real axis. The pole structures of symmetries IV, V, and VII (see Table I) are similar, but pole pairs are also possible in the upper half-plane.

correspond to genuinely distinct properties. In the following section we demonstrate this fact with potentials that are either purely parity pseudo-Hermitian (and not PT symmetrical) or time reversal invariant but not Hermitian.

IV. SEPARABLE POTENTIALS

In order to illustrate and test the theoretical concepts that we have discussed, in particular, the symmetrical configuration of poles with respect to the imaginary axis in the complex momentum plane for certain Hamiltonian symmetries, we use some solvable toy models consisting of rank 1 separable potentials. Separable potentials are quite useful models as a solvable approximation to realistic ones, in particular, in nuclear, atomic, and molecular physics [36]. Often they lead to explicit expressions for wave functions or scattering amplitudes, so they are used to test concepts and new methods. They are also instrumental in learning about different dynamical phenomena (for example, transient effects, short-time and long-time behavior, or anomalous decay laws) and their relation to complex-plane singularities [37–40]. Their simplest version takes the form $|\chi\rangle V_0\langle\chi|$ for some χ. In particular, with a complex V_0, they have been used to examine anomalous (negative) time delays caused by crossing of zeros of the S-matrix eigenvalues or S-matrix elements across the momentum real axis [41].

In this work we consider the simple structure $V = V_0|\phi\rangle\langle\chi|$, with V_0 (potential strength) real and conveniently chosen functions ϕ, χ. The aim of this section is to demonstrate the formal results of the previous section without attempting to simulate any specific systems, but we note that separable, NH potentials are instrumental to model nuclear reactions, in particular, by increasing the rank (number of separable terms) [42]. Separable NH potentials also provide solvable approximations to nonlocal NH potentials that arise naturally in quantum optics to describe the interaction of a ground-state atom with a laser beam [24]. In passing we also note some interesting phenomena that may be studied in more detail elsewhere, such as pole collisions, crossings of the real axis, or diodic (Maxwell demon) behavior with asymmetrical transmission for right-left incidence.

From the stationary Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, the eigenvalues of separable potentials may be found by solving

$$Q_0(E)V_0 = 1, \tag{20}$$

where $Q_0(E) = \langle\chi|(E - H_0)^{-1}|\phi\rangle$ and $H_0 = p^2/(2m)$. Moreover, for a separable potential, the transition operator T_{op} can be written (see Appendix C) as

$$T_{\mathrm{op}} = \frac{V_0}{1 - V_0 Q_0(E)}|\phi\rangle\langle\chi|. \tag{21}$$

Since all scattering amplitudes in S are simply related to matrix elements of T_{op} in momentum representation [see Eq. (A6)], solutions to Eq. (20) provide their core singularities (independent of the representation [38]). Once $Q_0(E)$ is calculated, the transmission and reflection amplitudes can be found from (A6) using the momentum representation of $|\phi\rangle$ and $|\chi\rangle$.

In the following subsections we build a Hamiltonian with symmetry V (time reversal) and another one with symmetry IV (parity pseudohermicity) and illustrate the symmetries of the S matrix poles in the momentum complex plane.

A. Time-reversal symmetric potential

We start with an example of a separable potential which only satisfies symmetry V (apart from the trivial symmetry I). The normalized vector $|\chi\rangle$ is given in position and momentum representation as

$$\langle x|\chi\rangle = \sqrt{\frac{a}{\hbar}}e^{-a|x|/\hbar}, \quad \langle p|\chi\rangle = \sqrt{\frac{2a^3}{\pi}}\frac{1}{p^2 + a^2}. \tag{22}$$

We choose $|\phi\rangle$ similarly as

$$\langle x|\phi\rangle = \sqrt{\frac{2ab}{\hbar(a+b)}}\begin{cases} e^{-bx/\hbar}, & x > 0,\\ e^{ax/\hbar}, & x < 0,\end{cases}$$

$$\langle p|\phi\rangle = \sqrt{\frac{ab}{\pi(a+b)}}\frac{a+b}{(p+ia)(p-ib)}. \tag{23}$$

The real and positive parameters $\hbar/a$ and $\hbar/b$ determine the width of the potential functions in coordinate representation. b is chosen different from a to introduce a right-left asymmetry in $\langle x|\phi\rangle$. In coordinate representation the potential is given as

$$\langle x|V|y\rangle = V_0\sqrt{\frac{2ba^2}{\hbar^2(a+b)}}\begin{cases} e^{-(a|y|+bx)/\hbar}, & x > 0,\\ e^{a(x-|y|)/\hbar}, & x < 0.\end{cases} \tag{24}$$

Clearly the potential is always even in y, and in the limiting case where $a = b$, it is also even in x. For $a = b$, the potential will satisfy parity symmetry (III) and also PT symmetry (VII), without asymmetric transmission or reflection.

We define first a complex momentum $q = \sqrt{2mE}$ (for complex E) with positive imaginary part. To calculate $Q_0(q)$ explicitly we use a closure relation in momentum representation and complex contour integration around the poles at ia, q, and ib. The result is then analytically continued to the whole q plane,

$$Q_0(q)/m = -\frac{i\sqrt{2b}[2a(a+b)^2 - q^2(3a+b) - iq(2a+b)(3a+b)]}{q(a+b)^{3/2}(a-iq)^2(b-iq)}, \tag{25}$$

with which we may calculate the transmission and reflection amplitudes. The four roots of Eq. (20) are the core poles.

Using m, V_0, and $\hbar$ we define the length and momentum scales $L_0 = \hbar/\sqrt{mV_0}$ and $p_0 = \sqrt{mV_0}$. In Fig. 2(a), we can see the trajectory of the S-matrix core poles [zeros of $1 - V_0Q_0(q)$] for varying V_0. Note the bound state for $V_0 < 0$ and collisions of the eigenvalue pairs around $V_0 = 0$. In Figs. 2(b) and 2(c), where V_0 is positive and a or b is varied, there are two virtual states and one resonance-antiresonance pair. In all cases the symmetry of the poles about the imaginary axis, which corresponds to real energies or complex-conjugate pairs of energies, is evident. For larger values of the a or b parameters (not shown) the pair collides so that all poles end up as virtual states.

Figure 3 depicts the associated transmission and reflection coefficients (square moduli of the amplitudes) as functions of the momentum p. $|R^l(p)| = |R^r(p)|$ for all p due to symmetry V [23]. The coefficients can be greater than 1, in contrast to the Hermitian case.

B. Parity pseudo-Hermitian potential

As the second example we consider a separable potential which only fulfills symmetry IV. The normalized vector $|\chi\rangle$ in position and momentum representation is

$$\langle x|\chi\rangle = \sqrt{\tfrac{a}{\hbar}}\begin{cases} e^{-(a+ib)x/\hbar}, & x > 0,\\ e^{ax/\hbar}, & x < 0,\end{cases}$$

$$\langle p|\chi\rangle = \sqrt{\tfrac{a}{2\pi}}\tfrac{2a+ib}{(p+ia)(p+b-ia)}, \tag{26}$$

where $a > 0$ and b is real. We choose $|\phi\rangle$ as

$$\langle x|\phi\rangle = \sqrt{\tfrac{a}{\hbar}}\begin{cases} e^{-ax/\hbar}, & x > 0,\\ e^{(a+ib)x/\hbar}, & x < 0,\end{cases}$$

$$\langle p|\phi\rangle = \sqrt{\tfrac{a}{2\pi}}\tfrac{2a+ib}{(p-ia)(p-b+ia)}, \tag{27}$$

where $\hbar/a$ gives, as before, the width in coordinate representation. The potential functions in coordinate representation become asymmetrical because of the imaginary terms ib in

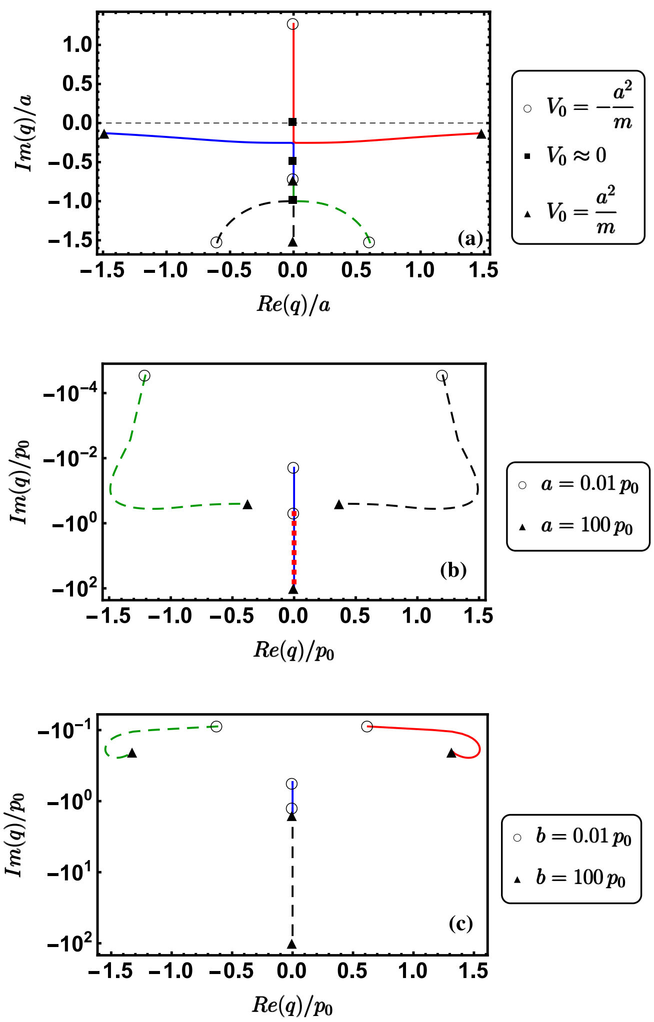

FIG. 2. Poles and pole trajectories of the time-reversal symmetric potential (24) for (a) varying V_0 with $a = 2b$; (b) varying a with $b = 0.5\,p_0$, $V_0 > 0$; and (c) varying b with $a = p_0$, $V_0 > 0$. At pole collisions we connect each of the incoming trajectories with a different emerging trajectory but the choice of outgoing branch is arbitrary since the two colliding poles lose their identity.

the exponent added only on one side. This term leads to oscillations in real and imaginary parts. In momentum representation b appears as a real shift in the position of one of the poles. In coordinate representation the potential is

$$\langle x|V|y\rangle = \frac{aV_0}{\hbar}\begin{cases} e^{-[a(x+y)-iby]/\hbar}, & x>0,\ y>0,\\ e^{a(y-x)/\hbar}, & x>0,\ y<0,\\ e^{[a(x-y)+ib(x+y)]/\hbar}, & x<0,\ y>0,\\ e^{[a(x+y)+ibx]/\hbar}, & x<0,\ y<0.\end{cases} \tag{28}$$

The case $b = 0$ implies that the potential is real and hence satisfies time-reversal symmetry (V) with equal reflection amplitudes (as in the previous case) and, also, symmetry VIII.

By calculating Q_0 again explicitly using complex contour integration around the poles at $-q$, $-b - ia$, and $b - ia$, we get that

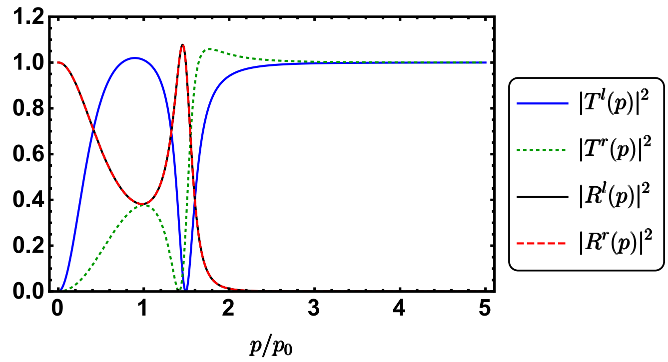

FIG. 3. Transmission and reflection coefficients of the time-reversal symmetric potential (24) with $a = p_0$, $b = 0.5p_0$, and $V_0 > 0$.

$$Q_0(q)/m = \frac{8a^2q^3 - 4a^2q(10a^2+b^2) - ia(4a^2+b^2)^2 + 32ia^3q^2}{q(4a^2+b^2)(a-iq)^2[b^2+(a-iq)^2]}. \tag{29}$$

Equation (20) has five roots in this case constituting core poles of the S-matrix elements.

Figure 4 depicts the trajectories of these poles for varying a, b, or V_0. As for the previous potential, the poles are symmetric with respect to the imaginary axis. In Fig. 4(a) there is a single bound state for $V_0 < 0$, while for positive values there are a resonance-antiresonance pair and a pair of virtual states. There are collisions of eigenvalues for values of V_0 close to 0. In Fig. 4(b) two complex-conjugate (bound) eigenvalues cross the real axis and become a resonance-antiresonance pair. At the exact point where the eigenvalues are on the real axis, the scattering amplitudes diverge, however, the eigenvalues of the S matrix do not, since divergences of the left and right amplitudes cancel each other. For $a \approx 4.55p_0$ a resonance-antiresonance pair collides and becomes a pair of virtual states. In Fig. 4(c) another crossing of the real axis takes place, but in this case when decreasing b.

Figure 5 depicts the associated transmission and reflection coefficients as functions of the momentum p. The eigenvalues are not always equal since parity pseudohermicity does not imply any strict restriction to them [23]. For large momenta, i.e., $p \gg \sqrt{2}p_0$, the potential is transparent, giving $T^l, T^r \approx 1$. For $p \approx 1.5p_0$ the right incidence transmission has a pronounced peak. Compared with 4(c), we note that the values of the potential parameters and the momentum are close to those for which the real axis crossing takes place. Around $p = 0.6p_0$ the potential acts as an asymmetric transmitter [23].

V. CONCLUSION

In this paper we have studied some aspects of the scattering of a structureless particle in one dimension by generally nonlocal and non-Hermitian potentials. Conditions that were found for discrete Hamiltonians to imply conjugate pairs of discrete eigenenergies (pseudohermiticity with respect to a linear operator or commutativity of H with an antilinear

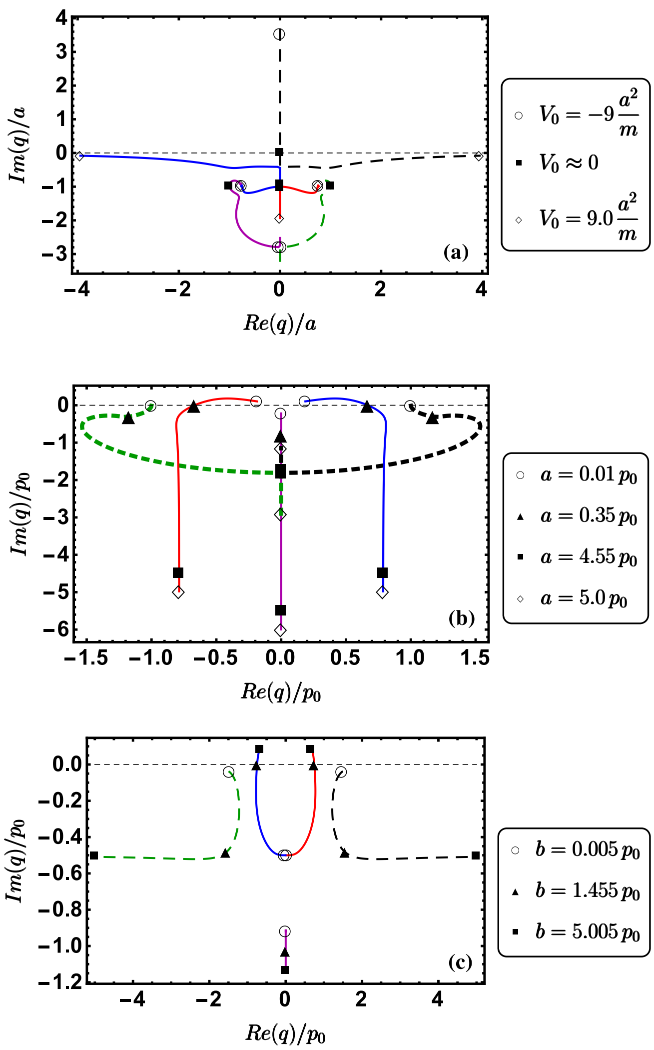

FIG. 4. Poles and pole trajectories for the parity pseudo-Hermitian potential (28) (a) varying V_0 with $a = b$; (b) varying a with $b = p_0$, $V_0 > 0$; and (c) varying b with $a = 0.5\,p_0$, $V_0 > 0$.

operator [25,26,43]) can in fact be extended to scattering Hamiltonians in the continuum, implying symmetry relations not just for bound-state eigenvalues but also for complex poles of the S matrix. Specifically the poles of S-matrix eigenvalues

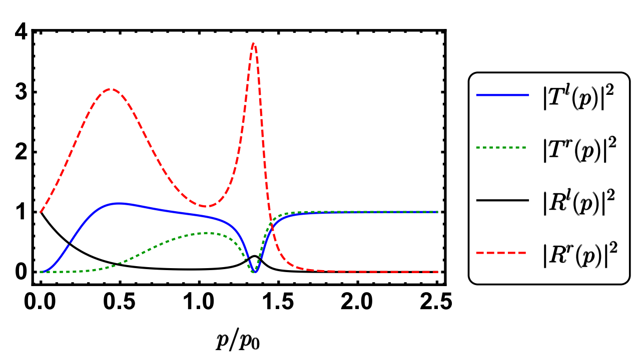

FIG. 5. Transmission and reflection coefficients for $a = b = 0.5p_0$ and $V_0 > 0$.

are symmetrically located with respect to the imaginary axis, also in the lower momentum plane, so that resonances and antiresonance energies are conjugate pairs as well. In terms of the eight possible Hamiltonian symmetries associated with Klein's group of A operators (unity, parity, time reversal, and PT) and their commutation or pseudohermiticity with H, the symmetrical disposition of the poles applies to four of them, which include hermiticity and PT symmetry. Potential models and pole motions are provided for the two other nontrivial symmetries: time-reversal symmetry and parity pseudohermiticity.

The study contributes to deepen our understanding of asymmetric scattering (with different responses for left and right incidence) beyond the much studied PT-symmetric potentials. This work opens interesting perspectives in atomic, molecular, and optical physics, where much activity on asymmetric scattering, mostly via optical devices, is currently being carried out. Moreover, asymmetric devices such as rectifiers, Maxwell demons, and diodes will be fundamental to develop quantum technologies and quantum information. For future work we plan to consider more complicated systems including internal states, as well as physical realizations of the different symmetries in quantum optical systems.

ACKNOWLEDGMENTS

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APPENDIX A: REVIEW OF SCATTERING THEORY FORMALISM

A detailed overview of scattering theory can be found in [44], and its extension to NH systems in [3]. Scattering theory describes the interaction of an incoming wave packet with a localized potential. In general, the spectrum of scattering Hamiltonians (as defined at the beginning of Sec. II) has both a discrete part and a continuum with real, positive energies. The eigenstates of the continuous spectrum are constructed by the action on plane waves of the Möller operators $|p^{\pm}\rangle = \Omega_{\pm}|p\rangle$ and $|\widehat{p}^{\pm}\rangle = \widehat{\Omega}_{\pm}|p\rangle$, where

$$\begin{aligned} \Omega_{+} &= \lim_{t\to-\infty} e^{iHt/\hbar}e^{-iH_0t/\hbar}, \quad & \Omega_{-} &= \lim_{t\to\infty} e^{iH^{\dagger}t/\hbar}e^{-iH_0t/\hbar}, \\ \widehat{\Omega}_{+} &= \lim_{t\to-\infty} e^{iH^{\dagger}t/\hbar}e^{-iH_0t/\hbar}, \quad & \widehat{\Omega}_{-} &= \lim_{t\to\infty} e^{iHt/\hbar}e^{-iH_0t/\hbar}, \end{aligned} \tag{A1}$$

and a regularization of the limit is implied (see, e.g., [3]). The Möller operators satisfy the isometry relation $\widehat{\Omega}_{\pm}^{\dagger}\Omega_{\pm} = 1$ and the intertwining relations $H\Omega_{+} = \Omega_{+}H_0$ and $H^{\dagger}\Omega_{-} = \Omega_{-}H_0$. By using the intertwining relations, it is easy to see that $|p^{+}\rangle$ and $|\widehat{p}^{-}\rangle$ are right eigenvectors of H, while $|\widehat{p}^{+}\rangle$ and $|p^{-}\rangle$ are left eigenvectors of H, all with positive energy $E_p = p^2/2m$. In the following we assume that the Hamiltonian admits a basis of biorthonormal right-left eigenstates

TABLE II. Transformation rules of the Möller and scattering operators under symmetries or pseudo-symmetries with linear or antilinear operators.

	A linear	A antilinear
$AH = HA$	$A\Omega_\pm = \Omega_\pm A$ $AS = SA$	$A\Omega_\pm = \widehat{\Omega}_\mp A$ $AS = \widehat{S}^\dagger A$
$AH = H^\dagger A$	$A\Omega_\pm = \widehat{\Omega}_\pm A$ $AS = \widehat{S}A$	$A\Omega_\pm = \Omega_\mp A$ $AS = S^\dagger A$

$\{|\psi_n\rangle, |\phi_a\rangle\}$ with energies E_n satisfying $\langle\phi_n|\psi_m\rangle = \delta_{n,m}$ for the discrete part. The stationary scattering states are also biorthonormal, i.e., $\langle\widehat{p}^+|q^+\rangle = \langle\widehat{p}^-|q^-\rangle = \delta(p-q)$, and together with the eigenstates of the discrete spectrum they give the resolution of the identity

$$\begin{aligned} 1 &= \sum_n |\psi_n\rangle\langle\phi_n| + \int_{-\infty}^{\infty} dp\, |p^+\rangle\langle\widehat{p}^+| \\ &= \sum_n |\psi_n\rangle\langle\phi_n| + \int_{-\infty}^{\infty} dp\, |\widehat{p}^-\rangle\langle p^-|. \end{aligned} \tag{A2}$$

There is no degeneracy in the discrete spectrum of 1D systems, whereas the continuum is doubly degenerate, e.g., with continuum eigenfunctions incident from the right or the left. We explicitly make use of this property in what follows. Using the resolution of the identity in terms of discrete eigenstates and the stationary scattering states, the Hamiltonian can be expanded as

$$H = \sum_n E_n|\psi_n\rangle\langle\phi_n| + \frac{1}{2m}\int_{-\infty}^{\infty} dp\, p^2|p^+\rangle\langle\widehat{p}^+|. \tag{A3}$$

We call the first and the second terms in (A3) the discrete, H_d, and continuous, H_c, parts of the Hamiltonian, respectively. A central object is the scattering operator (or matrix) $S \equiv \Omega_-^\dagger\Omega_+$ for scattering processes by H and $\widehat{S} \equiv \widehat{\Omega}_-^\dagger\widehat{\Omega}_+$ for $H^\dagger$. Unhatted quantities refer to scattering by H, while hatted quantities refer to scattering by its Hermitian conjugate $H^\dagger$. The scattering operator gives the probability of an incident state $|\psi_{\rm in}\rangle$ to be scattered (by H or $H^\dagger$) into a state $|\psi_{\rm out}\rangle$ as $|\langle\psi_{\rm out}|S|\psi_{\rm in}\rangle|^2$ or $|\langle\psi_{\rm out}|\widehat{S}|\psi_{\rm in}\rangle|^2$. Although the scattering operator is not unitary for NH Hamiltonians, S and $\widehat{S}$ obey the generalized unitarity relation $\widehat{S}^\dagger S = S\widehat{S}^\dagger = 1$, which collapses to the usual unitarity condition ($S = \widehat{S}$) if $H = H^\dagger$. If the Hamiltonian is symmetric or pseudo-Hermitian with respect to a linear or antilinear operator A, the Möller and scattering operators transform according to the intertwining relations in Table II. The intertwining relations of the Möller operators give the transformation rules for scattering states under A and provide interesting relations between the different transmission and reflection coefficients.

Also relevant to scattering theory is the transition operator, which is defined as

$$T_{\rm op}(E) = V + VG(E)V, \tag{A4}$$

where $G(E) = (E-H)^{-1}$ is Green's operator. The transition operator satisfies $T_{\rm op}^\dagger(z) = \widehat{T}_{\rm op}(z^*)$ and its matrix elements in momentum representation are related to the scattering operator by

$$\langle p|S|p'\rangle = \delta(p-p') - 2i\pi\delta(E_p - E_{p'})\langle p|T_{\rm op}(+)|p'\rangle, \tag{A5}$$

where $T_{\rm op}(\pm)|p'\rangle = \lim_{\epsilon\to 0^+} T_{\rm op}(E_p \pm i\epsilon)|p'\rangle$. This operator can then be used to define the scattering amplitudes for real p as

$$\begin{aligned} R^l(p) &= -\frac{2\pi i m}{p}\langle -p|T_{\rm op}(\mathrm{sign}(p))|p\rangle, \\ T^l(p) &= 1 - \frac{2\pi i m}{p}\langle p|T_{\rm op}(\mathrm{sign}(p))|p\rangle, \\ R^r(p) &= -\frac{2\pi i m}{p}\langle p|T_{\rm op}(\mathrm{sign}(p))|-p\rangle, \\ T^r(p) &= 1 - \frac{2\pi i m}{p}\langle -p|T_{\rm op}(\mathrm{sign}(p))|-p\rangle, \end{aligned} \tag{A6}$$

where $R^{l,r}$ is the left-right reflection amplitude and $T^{l,r}$ is the left-right transmission amplitude. We assume that the amplitudes admit analytic continuations. The generalized unitarity relation of the scattering operators give the following set of equations for the amplitudes

$$\begin{aligned} \widehat{T}^l(p)T^{l*}(p) + \widehat{R}^l(p)R^{l*}(p) &= 1, \\ \widehat{T}^r(p)T^{r*}(p) + \widehat{R}^r(p)R^{r*}(p) &= 1, \\ \hat{T}^{l*}(p)R^r(p) + T^r(p)\widehat{R}^{l*}(p) &= 0, \\ T^l(p)\widehat{R}^{r*}(p) + \widehat{T}^{r*}(p)R^l(p) &= 0, \end{aligned} \tag{A7}$$

where p is taken to be real and nonnegative. The Dirac deltas in Eq. (A5) make clear that the S matrix only connects momentum eigenstates having the same kinetic energy. Factoring out the Dirac delta of energy using $\delta(p-p') = \frac{|p|}{m}\delta(E_p - E_{p'})\delta_{pp'}$ ($\delta_{pp'}$ is to be understood as a Kronecker delta of the signs of the momenta), we can write $\langle p|S|p'\rangle = \frac{|p|}{m}\delta(E_p - E_{p'})\langle\mathbf{p}|\mathsf{S}|\mathbf{p}'\rangle$ in terms of the 2D vectors $|\mathbf{p}\rangle \equiv (1,0)^T$ and $|-\mathbf{p}\rangle \equiv (0,1)^T$, which correspond to the states $|p\rangle$ and $|-p\rangle$ for $p > 0$ [3]. The previous relation defines the on-the-energy-shell S matrix as

$$\begin{aligned} \langle\mathbf{p}|\mathsf{S}|\mathbf{p}'\rangle &= \delta_{pp'} - \frac{2i\pi m}{|p|}\langle p|T_{op}(+)|p'\rangle \\ &\Downarrow \\ \mathsf{S} &= \begin{pmatrix} T^l(p) & R^r(p) \\ R^l(p) & T^r(p)\end{pmatrix}. \end{aligned} \tag{A8}$$

$\widehat{\mathsf{S}}$ can be defined similarly. The on-the-energy-shell scattering matrix S inherits the generalized unitarity relation of the scattering operator S, i.e., $\widehat{\mathsf{S}}^\dagger\mathsf{S} = \mathbb{1}$. Equation (A7) is just this generalized unitarity relation written for all matrix elements.

APPENDIX B: ALTERNATIVE FORMULATION OF *A*-PSEUDO-HERMITIAN SYMMETRIES AS ORDINARY (COMMUTING) SYMMETRIES

Symmetry relations like (2) (for A either linear or antilinear) may also be expressed as ordinary (commuting) symmetries, generalizing for scattering Hamiltonians the work in [25], [26], and [43]. In other words, for a Hamiltonian H and a linear Hermitian (antilinear Hermitian) operator A satisfying (2) we can find an antilinear (linear) operator B that commutes with H. In this Appendix we explicitly construct the operators B from the Hamiltonian for A both linear and antilinear in the first and second sections, respectively.

Let us assume for now that besides A (linear or antilinear) there exists an invertible and Hermitian antilinear operator τ that also satisfies (2). With A and τ let us define the operator $B = A^{-1}\tau$, which will be antilinear (linear) for A linear (antilinear). As defined, B commutes with the Hamiltonian, because

$$\begin{aligned} BH &= A^{-1}\tau H = A^{-1}H^{\dagger}\tau \\ &= HA^{-1}\tau = HB. \end{aligned} \tag{B1}$$

B is not generally Hermitian unless τ commutes with A^{-1}.

The main task to define B is to find the antilinear operator τ that satisfies (2). This can be achieved if the eigenvectors of the Hamiltonian and its adjoint form bases of the Hilbert space that are biorthonormal. In [26] the expression of τ for a discrete spectrum (with no degeneracy) is found as

$$\tau_d|\zeta\rangle = \sum_n \langle\zeta|\phi_n\rangle|\phi_n\rangle, \tag{B2}$$

where the d subscript indicates that the Hamiltonian has a discrete spectrum. The action of the operator in Eq. (B2) on a vector in an eigenspace amounts to complex conjugation of its coordinate representation. τ_d is clearly antilinear, Hermitian (for antilinear operators hermicity is defined as $\langle\chi|\tau_d\zeta\rangle = \langle\zeta|\tau_d\chi\rangle$), and invertible. It can be checked that the relation $\tau_d H = H^{\dagger}\tau_d$ is satisfied.

To generalize this to Hamiltonians whose spectrum includes a continuous part, we have to build an antilinear operator τ that acts in both subspaces, $\mathcal{H}_d$ and $\mathcal{H}_c$, which are, respectively, spanned by the eigenfunctions associated with the discrete (point) and continuous spectra of the Hamiltonian. We propose to take $\tau = \tau_d + \tau_c$. The operators τ_d and τ_c act on complementary subspaces of the Hilbert space: while τ_d maps $\mathcal{H}_d$ to $\mathcal{H}_d$ and annihilates states in $\mathcal{H}_c$, τ_c maps $\mathcal{H}_c$ to $\mathcal{H}_c$ and annihilates states in $\mathcal{H}_d$. Specifically, we take τ_d to be given by Eq. (B2) with n denoting the eigenvectors of the Hamiltonian associated with the discrete part of the spectrum. To construct τ_c, note that to satisfy $\tau H = H^{\dagger}\tau$ [Eq. (2)] it has to transform right-scattering eigenvectors into some linear combination of left-scattering eigenvectors in the same energy shell. This is so because

$$H^{\dagger}\tau|p^+\rangle = \tau H|p^+\rangle = \tau E_p|p^+\rangle = E_p\tau|p^+\rangle. \tag{B3}$$

To fulfill the last requirement we set

$$\tau_c|\zeta\rangle = \int_{-\infty}^{\infty} dp[C_+(p)\langle\zeta|\widehat{p}^+\rangle|\widehat{p}^+\rangle + C_-(p)\langle\zeta|\widehat{p}^+\rangle|-\widehat{p}^+\rangle], \tag{B4}$$

where $C_+(p)$ and $C_-(p)$ are complex coefficients. It is straightforward to check that $\tau_c|p^+\rangle = C_+(p)|\widehat{p}^+\rangle + C_-(p)|-\widehat{p}^+\rangle$. The operator in (B4) is clearly antilinear because of the antilinearity of the inner product with respect to its first argument. Hermicity of τ requires $C_-(p) = C_-(-p)$. The condition that τ must be invertible restricts the coefficients in Eq. (B4) further. Consider the *on-shell* representation of τ_c, $\langle p^+|\tau q^+\rangle = \frac{|p|}{m}\delta(E_p - E_q)\mathsf{C}_{p,q}$, with $\mathsf{C}_{p,q} \equiv \delta_{p,q}C_+(q) + \delta_{p,-q}C_-(q)$, or in matrix form,

$$\mathsf{C}(p) = \begin{pmatrix} C_+(p) & C_-(p) \\ C_-(p) & C_+(-p) \end{pmatrix}. \tag{B5}$$

Since τ has to be invertible, $\mathsf{C}(p)$ must be invertible as well. This implies $C_+(p)C_+(-p) - C_-(p)C_-(p) \neq 0$.

In the following sections we construct expressions for B: in Sec. 1 for A linear and in Sec. 2 for A antilinear.

1. Pseudohermicity with linear operators

In [25,26], and [43] it is shown that pseudo-Hermitian Hamiltonians, i.e., those satisfying (2) for $A = \eta$ with η a Hermitian and invertible linear operator, possess an energy spectrum whose complex eigenvalues come in complex-conjugate pairs. Moreover, the eigenspaces associated with the eigenvalues E and E^* have the same degeneracy and η maps one to the other. Conversely, if the complex part of the spectrum of H contains only complex-conjugate pairs, it can be shown that there exists an η for which the Hamiltonian satisfies (2). These results hold for a general class of diagonalizable Hamiltonians with a discrete spectrum. For these Hamiltonians we can identify η with

$$\eta_d = \sum_{n_0}|\phi_{n_0}\rangle\langle\phi_{n_0}| + \sum_n[|\phi_{n_-}\rangle\langle\phi_{n_+}| + |\phi_{n_+}\rangle\langle\phi_{n_-}|], \tag{B6}$$

where the states $|\psi_{n_0}\rangle$ ($|\phi_{n_0}\rangle$) correspond to the right (left) eigenstates of H with real energy E_{n_0}. $|\psi_{n+/n-}\rangle$ ($|\phi_{n+/n-}\rangle$) correspond to the right (left) eigenvectors whose eigenvalue $E_{n+/n-}$ has a positive/negative imaginary part. This gives $\eta_d|\psi_{n_0}\rangle = |\phi_{n_0}\rangle$, $\eta_d|\psi_{n_+}\rangle = |\phi_{n_-}\rangle$, and $\eta_d|\psi_{n_-}\rangle = |\phi_{n_+}\rangle$. Clearly η_d is compatible with pseudohermicity since it maps right eigenvectors associated with eigenvalue E to left eigenvectors with eigenvalue E^* and the pseudohermicity relation, (2), is satisfied. To generalize (B6) for a scattering Hamiltonian we must add an additional term η_c which acts on the subspace of scattering states and is compatible with the hermiticity and invertibility of $\eta = \eta_d + \eta_c$. Since η should transform the right scattering states into left ones in the same energy shell, $\eta_c|p^+\rangle$ should be a linear combination of both $|\widehat{p}^+\rangle$ and $|-\widehat{p}^+\rangle$. Accordingly, we propose

$$\eta_c = \int_{-\infty}^{\infty} dp\,[\Lambda_+(p)|\widehat{p}^+\rangle\langle\widehat{p}^+| + \Lambda_-(p)|-\widehat{p}^+\rangle\langle\widehat{p}^+|], \tag{B7}$$

where $\Lambda_+(p)$, $\Lambda_-(p)$ are complex coefficients depending on the momentum p. Hermicity of η requires $\Lambda_+(p) \in \mathbb{R}$ and $\Lambda_-^*(p) = \Lambda_-(-p)$.

Since η_c connects scattering states with the same energy it admits the *on-shell* representation $\langle q^+|\eta_c|p^+\rangle = \frac{|p|}{m}\delta(E_q - E_p)\Lambda_{q,p}(p)$, with $\Lambda_{q,p}(p) \equiv \delta_{q,p}\Lambda_+(p) + \delta_{q,-p}\Lambda_-(p)$, or in matrix form

$$\Lambda(p) = \begin{pmatrix} \Lambda_+(p) & \Lambda_-^*(p) \\ \Lambda_-(p) & \Lambda_+(-p) \end{pmatrix}. \tag{B8}$$

Since η has to be invertible, this implies that the determinant of $\mathsf{A}(p)$ should not vanish, i.e., $\Lambda_+(p)\Lambda_+(-p) -$

$\Lambda_-(p)\Lambda_-^*(p) \neq 0$. The inverse of η is then $\eta^{-1} = \eta_d^{-1} + \eta_c^{-1}$ with

$$\eta_d^{-1} = \sum_{n_0} |\psi_{n_0}\rangle\langle\psi_{n_0}| + \sum_n [|\psi_{n_+}\rangle\langle\psi_{n_-}| + |\psi_{n_-}\rangle\langle\psi_{n_+}|], \tag{B9}$$

$$\eta_c^{-1} = \int_{-\infty}^{\infty} dp\, [\Lambda_+^{(-1)}(p)|p^+\rangle\langle p^+| + \Lambda_-^{(-1)}(p)|-p^+\rangle\langle p^+|], \tag{B10}$$

where the complex coefficients $\Lambda_\pm^{(-1)}(p)$ are taken from the inverse of $\Lambda(p)$,

$$\Lambda^{-1}(p) = \begin{pmatrix} \Lambda_+^{(-1)}(p) & \Lambda_-^{(-1)*}(p) \\ \Lambda_-^{(-1)}(p) & \Lambda_+^{(-1)}(-p) \end{pmatrix}. \tag{B11}$$

Using the orthogonality between the subspace of discrete (bound) and scattering states we find the final expression for B:

$$\begin{aligned} B|\zeta\rangle &= \eta_d^{-1}\tau_d|\zeta\rangle + \eta_c^{-1}\tau_c|\zeta\rangle = \sum_{n_0}\langle\zeta|\phi_{n_0}\rangle|\psi_{n_0}\rangle \\ &+ \sum_n \langle\zeta|\phi_{n_+}\rangle|\psi_{n_-}\rangle + \sum_n \langle\zeta|\phi_{n_-}\rangle|\psi_{n_+}\rangle \\ &+ \int_{-\infty}^{\infty} dp\, \langle\zeta|\widehat{p}^+\rangle[\tilde{C}_+(p)|p^+\rangle + \tilde{C}_-(p)|-p^+\rangle], \end{aligned} \tag{B12}$$

with $\tilde{C}_\pm(p) = C_+(p)\Lambda_\pm^{(-1)}(p) + C_-(p)\Lambda_\mp^{(-1)}(-p)$. Note that the resulting operator B is antilinear.

2. Pseudohermicity with antilinear operators

In this section we consider the case where the operator A appearing in Eq. (2) is antilinear. In Ref. [26] this is called antipseudohermicity, but we do not use this terminology in order to avoid confusion with antihermicity ($H = -H^\dagger$). The effect of A on a right eigenvector of H is to transform it into its corresponding biorthonormal partner, i.e., the left eigenvector corresponding to the same energy:

$$\begin{gathered} H^\dagger A|\psi_n\rangle = AH|\psi_n\rangle = AE_n|\psi_n\rangle = E_n^* A|\psi_n\rangle \\ \Downarrow \\ A|\psi_n\rangle \propto |\phi_n\rangle. \end{gathered} \tag{B13}$$

A also admits a decomposition similar to Eq. (B2). The Hamiltonian satisfies Eq. (2) with respect to τ. One can check that $A^{-1}\tau$ is a linear symmetry of the Hamiltonian, $HA^{-1}\tau - A^{-1}\tau H = 0$. The expansion of A on the discrete and scattering basis is

$$\begin{aligned} A|\xi\rangle = \sum_n g_n \langle\xi|\phi_n\rangle|\phi_n\rangle + \int dp\, \langle\xi|\widehat{p}^+\rangle[G_+(p)|\widehat{p}^+\rangle \\ + G_-(p)|-\widehat{p}^+\rangle], \end{aligned} \tag{B14}$$

with $A|p^+\rangle = G_+(p)|\widehat{p}^+\rangle + G_-(p)|-\widehat{p}^+\rangle$ and $g_n = \langle\psi_n|A\psi_n\rangle$. As examples we have found the expressions of $B = A^{-1}\tau$ for $A_T = \Theta$ (time reversal) and $A_{\rm PT} = \Pi\Theta$ (PT). In both cases we have $A_T^{-1} = A_T$ and $A_{\rm PT}^{-1} = A_{\rm PT}$.

a. PT symmetry

The action of $B_{\rm PT} = A_{\rm PT}\tau$ on an arbitrary state is

$$\begin{aligned} B_{\rm PT}|\zeta\rangle = A_{\rm PT}\tau|\zeta\rangle = A_{PT}\bigg\{ \sum_n \langle\zeta|\phi_n\rangle|\phi_n\rangle \\ + \int dp\, [C_+(p)\langle\zeta|\widehat{p}^+\rangle|\widehat{p}^+\rangle \\ + C_-(p)\langle\zeta|\widehat{p}^+\rangle|-\widehat{p}^+\rangle]\bigg\}. \end{aligned} \tag{B15}$$

Using $A_{\rm PT}H = H^\dagger A_{\rm PT}$ and Table II we have $A_{\rm PT}|\widehat{p}^\pm\rangle = |\widehat{p}^\mp\rangle$. Note that the "−" right scattering states can be expressed in terms of the "+" right scattering states as

$$\begin{aligned} |\widehat{p}^-\rangle &= \int dq\, |q^+\rangle\langle\widehat{q}^+|\widehat{p}^-\rangle \\ &= \int dq\, |q^+\rangle\langle q|\widehat{\Omega}_+^\dagger\widehat{\Omega}_-|p\rangle \\ &= \int dq\, |q^+\rangle\langle q|\widehat{S}^\dagger|p\rangle \\ &= |p^+\rangle\langle p|\widehat{\mathsf{S}}^\dagger|p\rangle + |-p^+\rangle\langle -p|\widehat{\mathsf{S}}^\dagger|p\rangle. \end{aligned} \tag{B16}$$

With all this, the final form of $B_{\rm PT}$ is

$$\begin{aligned} B_{\rm PT} &= \sum_n (g_n^*)^{-1}|\psi_n\rangle\langle\phi_n| \\ &+ \int dp\, [\tilde{C}_+^*(p)|p^+\rangle\langle\widehat{p}^+| + \tilde{C}_-^*(p)|-p^+\rangle\langle\widehat{p}^+|], \end{aligned} \tag{B17}$$

with $C_\pm^*(p) = C_\pm^*(p)\langle\pm p|\widehat{\mathsf{S}}^\dagger|\pm p\rangle + C_\mp^*(p)\langle\pm p|\widehat{\mathsf{S}}^\dagger|\mp p\rangle$.

b. Time-reversal symmetry

For time-reversal symmetry,

$$\begin{aligned} B_T|\zeta\rangle = A_T\tau|\zeta\rangle = A_T\bigg\{ \sum_n \langle\zeta|\phi_n\rangle|\phi_n\rangle \\ + \int dp\, [C_+(p)\langle\zeta|\widehat{p}^+\rangle|\widehat{p}^+\rangle \\ + C_-(p)\langle\zeta|\widehat{p}^+\rangle|-\widehat{p}^+\rangle]\bigg\}. \end{aligned} \tag{B18}$$

Since the time-reversal operator satisfies relation (2) with the Hamiltonian, Table II implies $A_T|\widehat{p}^\pm\rangle = |-\widehat{p}^\mp\rangle$. The linear symmetry operator can be expressed as in Eq. (B17) but in this case $\tilde{C}_\pm^*(p) = C_\pm^*(p)\langle\pm p|\widehat{\mathsf{S}}^\dagger|\mp p\rangle + C_\mp^*(p)\langle\pm p|\widehat{\mathsf{S}}^\dagger|\pm p\rangle$.

APPENDIX C: PROPERTIES OF SEPARABLE POTENTIALS

For a separable potential $V = V_0|\phi\rangle\langle\chi|$, the transition operator becomes

$$T_{\rm op} = \alpha|\phi\rangle\langle\chi|, \tag{C1}$$

where $\alpha = V_0 + V_0^2\langle\chi|G(E)|\phi\rangle$. Then using the Lippmann-Schwinger equation we get that

$$\begin{aligned} T_{\mathrm{op}}(E) &= V + VG_0(E)T_{\mathrm{op}}(E) \\ &= [V_0 + \alpha V_0\langle\chi|G_0(E)|\phi\rangle]|\phi\rangle\langle\chi|, \end{aligned} \tag{C2}$$

where $G_0(E) = (E - H_0)^{-1}$ is the Green's operator for free motion. Solving for α now gives

$$\alpha = \frac{V_0}{1 - V_0\langle\chi|G_0(E)|\phi\rangle} = \frac{V_0}{1 - V_0Q_0(E)}. \tag{C3}$$

1. S-matrix eigenvalues

The eigenvalues for the S matrix are given by Eq. (12) in terms of the reflection and transmission amplitudes. For a separable potential, using Eq. (A6), we can simplify the transmission and reflection coefficients as

$$\begin{aligned} T^l &= 1 - \frac{2\pi im}{p}\alpha\phi(p)\chi^*(p), \\ T^r &= 1 - \frac{2\pi im}{p}\alpha\phi(-p)\chi^*(-p), \\ R^l &= -\frac{2\pi im}{p}\alpha\phi(-p)\chi^*(p), \\ R^r &= -\frac{2\pi im}{p}\alpha\phi(p)\chi^*(-p). \end{aligned} \tag{C4}$$

If we now define

$$\Gamma = \frac{2\pi im}{p}\alpha[\phi(p)\chi^*(p) + \phi(-p)\chi^*(-p)], \tag{C5}$$

we can write the eigenvalues as simply

$$S_j = 1 - \frac{\Gamma - (-1)^j\Gamma}{2}. \tag{C6}$$

Note that $S_2 = 1$ for all p. Clearly the following relation must also always hold for the reflection and transmission amplitudes,

$$T^l + T^r - T^lT^r + R^lR^r = 1. \tag{C7}$$

2. Uniqueness of the bound state

A separable potential can only have at most one bound state $|\psi_E\rangle$. In momentum representation,

$$\begin{aligned} \langle p|\psi_E\rangle &= \langle p|\frac{V_0}{E - H_0}|\phi\rangle\langle\chi|\psi_E\rangle \\ &= \frac{M}{p^2 - q_B^2}\langle p|\phi\rangle, \end{aligned} \tag{C8}$$

where $M = -2mV_0\langle\chi|\psi_E\rangle$ and $q_B^2 = 2mE < 0$. Suppose there is a second bound state $|\psi_{E'}\rangle$, with corresponding quantities M' and $q_{B'}^2$. Then

$$\langle\psi_{E'}|\psi_E\rangle = MM'\int_{-\infty}^{\infty} dp|\langle p|\phi\rangle|^2\frac{1}{p^2 - q_B^2}\frac{1}{p^2 - q_{B'}^2}. \tag{C9}$$

Since $MM' \neq 0$ and the integral is positive the overlap cannot be zero so there cannot be two bound states.

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[27] *S*-matrix poles of Hermitian Hamiltonians are symmetric in the complex momentum plane with respect to the imaginary axis (see Fig. 1). In the upper half-plane they are on the imaginary axis and represent bound states. In the lower half-plane they come in symmetrical resonance and antiresonance pairs and may also lie on the imaginary axis as "virtual states." A further symmetry is the occurrence of a 0 at the complex-conjugate

momentum of a given pole. These properties are well known for partial-wave scattering by spherical potentials but also hold for the S-matrix eigenvalues in 1D scattering [3]. For NH Hamiltonians the above pole and pole/zero symmetries do not hold in general.

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[30] Also, discrete Hamiltonian matrix models abound in many fields, for example, quantum optics, in which, rather than couplings among different "sites," there are couplings among states or levels. Thus a generalized concept of "nonlocality" may be applied as being equivalent to nonzero nondiagonal elements in the chosen basis. The non-Hermitian symmetry groups in these discrete models can be larger than the set of symmetries based on Eqs. (1) and (2) described here, which are constrained by the structure of H_0. Discrete model symmetries, interesting as they are, and with potential applications in condensed matter, optics, or quantum optics, lie beyond the scope of this work and require a deeper separate study.

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