Symmetries and invariants for non-Hermitian Hamiltonians

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We discuss Hamiltonian symmetries and invariants for quantum systems driven by non-Hermitian Hamiltonians. For time-independent Hermitian Hamiltonians, a unitary or antiunitary transformation \(AH \hat{A}^\dagger\) that leaves the Hamiltonian \(H\) unchanged represents a symmetry of the Hamiltonian, which implies the commutativity \([H, A] = 0\), and a conservation law, namely the invariance of expectation values of \(A\). For non-Hermitian Hamiltonians, \(H^\dagger\) comes into play as a distinct operator that complements \(H\) in generalized unitarity relations. The above description of symmetries has to be extended to include also \(A\)-pseudohermiticity relations of the form \(AH = H^\dagger A\). A superoperator formulation of Hamiltonian symmetries is provided and exemplified for Hamiltonians of a particle moving in one-dimension considering the set of \(A\) operators forming Klein’s 4-group: parity, time-reversal, parity\&time-reversal, and unity. The link between symmetry and conservation laws is discussed and shown to be more subtle for non-Hermitian than for Hermitian Hamiltonians.

I. INTRODUCTION

The intimate link between invariance and symmetry is well studied and understood for Hermitian Hamiltonians but non-Hermitian Hamiltonians pose some interesting conceptual and formal challenges. Non-Hermitian Hamiltonians arise naturally in quantum systems as effective interactions for a subsystem. These Hamiltonians may be proposed phenomenologically or may be found exactly or approximately by applying Feshbach’s projection technique to describe the dynamics in the subsystem [1, 2]. It is thus important to understand how common concepts for Hermitian Hamiltonians such as “symmetry”, “invariants”, or “conservation laws” generalize. A lightning review of concepts and formal relations for a time-independent Hermitian Hamiltonian \(H\) will be helpful as the starting point to address generalizations for a non-Hermitian \(H\). Unless stated otherwise, \(H\) is time-independent in the following. In quantum mechanics \(A\) (unitary or antiunitary) represents a symmetry of the Hamiltonian if

\[A^\dagger HA = H,\]  

so that

\[[H, A] = 0,\]  

and thus \(A\) (which we assume to be time-independent) represents also a conserved quantity,

\[⟨ψ(t), Aψ(t)⟩ = ⟨ψ(0), Aψ(0)⟩,\]  

where \(ψ(t) = U(t)ψ(0)\) is the time-dependent wave function satisfying the Schrödinger equation

\[i\hbar \partial_t |ψ(t)⟩ = H |ψ(t)⟩,\]  

and \(U(t) = e^{-iHt/\hbar}\) is the unitary evolution operator from 0 to \(t\), \(U(t)U^\dagger(t) = U^\dagger(t)U(t) = 1\). Backwards evolution in time from \(t\) to 0 is represented by \(U(−t) = U(t)^\dagger\) so that the initial state is recovered by a forward and backward sequence, \(U(t)^\dagger U(t)|ψ(0)⟩ = |ψ(0)⟩\).

Equation (4) is mostly significant for a linear \(A\). If \(A\) is antilinear only the modulus is relevant, as the result changes if we multiply the state by a unit modulus phase factor, \(ψ(0) → e^{iφ}ψ(0)\). This ambiguity does not mean at all that antilinear symmetries do not have physical consequences. They affect, for example, selection rules for possible transitions.

More generally, time-independent operators \(A\) satisfying (2), fulfill (3) without the need to be unitary or antiunitary, and represent also invariant quantities. A further property from (2) is that if \(|φ_E⟩\) is an eigenstate of \(H\) with (real) eigenvalue \(E\), then \(A|φ_E⟩\) is also an eigenstate of \(H\) with the same eigenvalue.

II. DUAL CHARACTER OF \(H\) AND \(H^\dagger\)

Defining \(\hat{U}(t) = e^{-iH^\dagger t/\hbar}\), we find the generalized unitarity relations \(U(t)\hat{U}^\dagger(t) = \hat{U}^\dagger U(t) = 1\). Backwards evolution with \(H^\dagger\) compensates the changes induced forwards by \(H\). Similar generalized unitarity relations exist for the...
scattering $S$ matrix (for evolution with $H$) and the corresponding $\hat{S}$ (for evolution with $H^\dagger$), with important physical consequences discussed e.g. in [3, 4].

Now consider the following two formal generalizations of the element $\langle \psi(t), A\psi(t) \rangle$ in Equation (4),

$$\langle e^{-iHt/\hbar}\psi(0), Ae^{-iHt/\hbar}\psi(0) \rangle = \langle \tilde{\psi}(t), A\psi(t) \rangle,$$

and the generalizations of (2)

$$AH = HA,$$

$$AH = H^\dagger A.$$  \hspace{2cm} (7)  

We name A pseudohermiticity of $H$. (This is here a formal definition that does not presupose any further property on $A$.) Up to normalization, which will be discussed in the following section, Equation (6) corresponds to the usual rule to define expectation values, whereas (5), where $|\phi_j\rangle$ is a right eigenstate of $H$ for $|A\rangle$ linear, or a left eigenstate of $H$ for $|A\rangle$ antilinear. As right and left eigenvectors must be treated on equal footing, since both are needed for the resolution, this argument points at a similar importance of the relations (4) and (5).

III. TIME EVOLUTION FOR NORMALIZED STATES

For a quantum system following the Schrödinger Equation (4) with $H$ non-Hermitian, in general the evolution will not be unitary and the norm $N_\psi(t) \equiv \langle \psi(t)|\psi(t) \rangle$ is not conserved. We shall assume the initial condition $N_\psi(0) = 1$. Using Equation (4), the rate of change of the norm is

$$\partial_t \langle \psi(t)|\psi(t) \rangle = \frac{1}{i\hbar} \langle \psi(t)|H - H^\dagger |\psi(t) \rangle \neq 0.$$  \hspace{2cm} (11)

**Expectation Values.** We now restrict the discussion to linear observables $A$. Since the state of the system is not normalized to 1 for $t > 0$, the expectation value formula has to take into account the norm explicitly,

$$\langle A \rangle (t) = \frac{\langle \psi(t)|A|\psi(t) \rangle}{\langle \psi(t)|\psi(t) \rangle}.$$  \hspace{2cm} (12)

Using Equations (4) and (11), the rate of change of the expectation value of $A$ is

$$\partial_t \langle A \rangle (t) = \frac{1}{i\hbar} \frac{\langle \psi(t)|\psi(t) \rangle (\langle \psi(t)|AH - H^\dagger A|\psi(t) \rangle - \langle \psi(t)|H - H^\dagger |\psi(t) \rangle (\langle \psi(t)|A|\psi(t) \rangle)}{\langle \psi(t)|\psi(t) \rangle^2}.$$  \hspace{2cm} (13)
For Hermitian Hamiltonians the commutation of $A$ and $H$ leaves the expectation values of $A$ invariant. For non-Hermitian Hamiltonians the symmetry Equation (8) applied to Equation (13) gives

$$\partial_t \langle A \rangle (t) = \frac{-1}{i\hbar} \frac{\langle \psi(t)|H - H^\dagger|\psi(t)\rangle \langle \psi(t)|A|\psi(t)\rangle}{\langle \psi(t)|\psi(t)\rangle^2}. \quad (14)$$

If we use Equations (11) and (12) in Equation (14),

$$\frac{\langle A \rangle}{\langle \psi(t)|\psi(t)\rangle} \partial_t \langle \psi(t)|\psi(t)\rangle = -\partial_t \langle A \rangle, \quad (15)$$

$$\langle A \rangle \langle \psi(t)|\psi(t)\rangle = \text{Constant}. \quad (16)$$

Applying the initial condition $\langle \psi(0)|\psi(0)\rangle = 1$,

$$\langle A \rangle (t) = \frac{\langle A \rangle (0)}{\langle \psi(t)|\psi(t)\rangle}, \quad (17)$$

so the expectation value of an $A$ that obeys $AH = H^\dagger A$, is simply rescaled by the norm of the wave function as it increases or decreases.

*Lower bound on the norm of the wave function.* The symmetry condition $AH = H^\dagger A$ may set lower bounds to the norm along the dynamical process. Consider a linear observable $A$ with real eigenvalues $\{a_i\}$ bounded by $\max\{|a_i|\}$. Then, the expectation values satisfy $|\langle A \rangle| \leq \max\{|a_i|\}$. If we use the result in (17) we get

$$\langle \psi(t)|\psi(t)\rangle \geq |\langle A \rangle (0)| / \max\{|a_i|\}. \quad (18)$$

Equation (18) bounds the norm of the state due to symmetry conditions. A remarkable case is parity pseudohermiticity, $\Pi H = H^\dagger \Pi$, where the parity operator acts on the position eigenstates as $\Pi |x\rangle = |-x\rangle$ and has eigenvalues $\{-1, 1\}$. Under this symmetry, Equation (18) gives

$$\langle \psi(t)|\psi(t)\rangle \geq |\langle \Pi \rangle (0)|, \quad (19)$$

where $\langle \Pi \rangle (0)$ is the expectation value of the state at $t = 0$.

**IV. GENERIC SYMMETRIES**

We postulate that both (7) and (8), for $A$ unitary or antiunitary, are symmetries of the Hamiltonian. A superoperator framework helps to understand why (8) also represents a symmetry. Let us define the superoperators $\mathcal{L}_A(\cdot) \equiv A^\dagger(\cdot)A$, $\mathcal{L}_1(\cdot) \equiv (\cdot)^\dagger$ and $\mathcal{L}_{A,1}(\cdot) \equiv \mathcal{L}_A(\mathcal{L}_1(\cdot)) = \mathcal{L}_1(\mathcal{L}_A(\cdot))$. For linear operators $B$ and a complex number $a$ they satisfy

$$\mathcal{L}_A(ab) = a\mathcal{L}_A(B), \quad \text{A unitary}, \quad (20)$$

$$\mathcal{L}_A(ab) = a^\ast \mathcal{L}_A(B), \quad \text{A antiunitary}, \quad (21)$$

$$\mathcal{L}_1(ab) = a^\ast \mathcal{L}_1(B), \quad (22)$$

$$\mathcal{L}_{A,1}(ab) = a^\ast \mathcal{L}_{A,1}(B), \quad \text{A unitary}, \quad (23)$$

$$\mathcal{L}_{A,1}(ab) = a\mathcal{L}_{A,1}(B), \quad \text{A antiunitary}. \quad (24)$$

As the product of two antilinear operators is a linear operator, the resulting operators (on the right hand sides) are linear in all cases, independently of the linearity or antilinearity of $A$. This should not be confused with the linearity or antilinearity of the superoperators $\mathcal{L}$ that may be checked by the invariance (for a linear superoperator) or complex conjugation (for an antilinear superoperator) of the constant $a$. Using the scalar product for linear operators $F$ and $G$,

$$\langle \langle F, G \rangle \rangle \equiv \text{Tr}(F^\dagger G), \quad (25)$$

we find the adjoints,

$$\mathcal{L}^\dagger_A(\cdot) = \mathcal{L}_{A^\dagger}(\cdot) \equiv A(\cdot)A^\dagger, \quad (26)$$

$$\mathcal{L}^\dagger_1(\cdot) = \mathcal{L}_1(\cdot), \quad (27)$$

$$\mathcal{L}^\dagger_{A,1}(\cdot) = \mathcal{L}_{A^\dagger,1}(\cdot), \quad (28)$$
asymmetrical devices such as diodes or rectifiers in quantum circuits \[9\].

Reflection or transmission amplitudes for right and left incidence, are relevant information to implement microscopic column may be classified as antiunitary (symmetries II, IV, V, and \( VI ) and unitary (symmetries I, III, VI, and \( VIII ) .

Operators commute. Moreover they are Hermitian and equal to their own inverses. The superoperators in the third order or momenta). \( H \)

Hamiltonian symmetries described by the eight relations of the second column. They amount to the invariance of the is diagonalizable, possibly with discrete and continuum parts. By inspection of Table \( I \), one finds a set of possible

\[
\langle\langle F, \mathcal{L}G \rangle\rangle = \langle\langle G, \mathcal{L}F \rangle\rangle^* \quad \text{for } \mathcal{L} \text{ linear and } \langle\langle F, \mathcal{L}^\dagger G \rangle\rangle = \langle\langle G, \mathcal{L}F \rangle\rangle \quad \text{for } \mathcal{L} \text{ antilinear.}
\]

All the above transformations are unitary or antunitary (in a superoperator sense), \( \mathcal{L}^\dagger = \mathcal{L}^{-1} \), and they keep “transition probabilities” among two states represented by density operators \( \rho_1 \) and \( \rho_2 \) invariant, namely

\[
\langle\langle \mathcal{L}\rho_1, \mathcal{L}\rho_2 \rangle\rangle = \langle\langle \rho_1, \rho_2 \rangle\rangle.
\]

Due to the Hermiticity of the density operators, \( \langle\langle \rho_1, \rho_2 \rangle\rangle \) is a real number (both for unitary or antunitary \( \mathcal{L} \)). This result is reminiscent of Wigner’s theorem, originally formulated for pure states \( [7] \), but considering a more general set of states and transformations.

We conclude that all of the above \( \mathcal{L} \) superoperators may represent symmetry transformations and, in particular, Hamiltonian symmetries if they leave the Hamiltonian invariant, namely, \( \mathcal{L}H = H \). The following section demonstrates this for the set of symmetry transformations that leave Hamiltonians for a particle in one dimension invariant, making use of transposition, complex conjugation, and inversion of coordinates or momenta.

As for the connection between symmetries and conservation laws, the results of the previous sections apply. It is possible to find quantities that on calculation remain invariant, but they are not necessarily physically significant.

### V. EXAMPLE OF PHYSICAL RELEVANCE OF THE RELATIONS \( AH = HA, AH = H^\dagger A \) AS SYMMETRIES

In this section we exemplify the above general formulation of Hamiltonian symmetries for Hamiltonians of the form \( H_0 + V \) corresponding to a particle of mass \( m \) moving in one dimension, where \( H_0 = P^2/(2m) \) is the kinetic energy, \( P \) the momentum operator, and \( V \) is a generic potential that may be non-Hermitian and non-local (non-local means that matrix elements in coordinate representation, \( \langle x|V|y \rangle \), may be non-vanishing for \( x \neq y \)). We assume that \( H \) is diagonalizable, possibly with discrete and continuum parts. By inspection of Table \( IV \) one finds a set of possible Hamiltonian symmetries described by the eight relations of the second column. They amount to the invariance of the Hamiltonian with respect to the transformations represented by the superoperators in the third column. In coordinate or momentum representation, see the last two columns, each symmetry amounts to the invariance of the potential matrix elements with respect to some combination of transposition, complex conjugation and inversion (of coordinates or momenta). \( (H_0 \) is invariant with respect to the eight transformations.)

The eight superoperators form the elementary abelian group of order eight \( [8] \), with a minimal set of three generators \( \mathcal{L}_1, \mathcal{L}_{II}, \mathcal{L}_\Theta \), from which all elements may be formed by multiplication (i.e., successive application). \( \Theta \) is the antilinear time-reversal operator. Note that no other transformation is possible that leaves the Hamiltonian invariant making only use of transposition, complex conjugation, inversion, and their combinations. The eight superoperators may also be found by the generating set \( \{ \mathcal{L}_A, \mathcal{L}_1 \} \), where \( A \) is one of the elements of Klein’s 4-group \( \{1, \Theta, II, \Theta I \} \). These four operators commute. Moreover they are Hermitian and equal to their own inverses. The superoperators in the third column may be classified as antunitary (symmetries II, IV, V, and VII) and unitary (symmetries I, III, VI, and VIII).

In \( [3] \) these symmetries are exploited to find selections rules that allow or disallow certain asymmetries in the reflection or transmission amplitudes for right and left incidence, a relevant information to implement microscopic asymmetrical devices such as diodes or rectifiers in quantum circuits \( [5] \).
VI. DISCUSSION

The relations between invariance and symmetry are often emphasized, but for non-Hermitian Hamiltonians, which occur naturally as effective interactions, they become more complex and subtle than for Hermitian Hamiltonians. We have discussed these relations for time-independent Hamiltonians.

For time-dependent Hamiltonians additional elements are needed. In 1969, Lewis and Riesenfeld [10] showed that the motion of a system subjected to time-varying forces admits a simple decomposition into elementary, independent motions characterized by constant values of some quantities (eigenvalues of the invariant). In other words, the dynamics is best understood, and is most economically described, in terms of invariants even for time-dependent Hamiltonians. In fact the powerful link between forces and invariants can be used in reverse order to inverse engineer from the invariant associated with some desired dynamics the necessary driving forces.

Time-dependent non-Hermitian Hamiltonians require a specific analysis and will be treated in more detail elsewhere. However we briefly advance here some important differences with the time-independent Hamiltonians. Invariants for Hermitian time-dependent Hamiltonians obey the invariance condition

\[
\frac{\partial I(t)}{\partial t} - \frac{1}{i\hbar}[H(t), I(t)] = 0,
\]

so that \( \frac{d}{dt}(\psi(t)|I(t)\rangle\langle I(t)|\psi(t)) = 0 \) for states \( \psi(t) \) that evolve with \( H(t) \) (we assume that the invariant is linear). In general the operator \( I(t) \) may depend on time and the invariant quantity is the expectation value \( \langle \psi(t)|I(t)\rangle\langle I(t)|\psi(t) \rangle \). In this context a Hamiltonian symmetry, defined by the commutativity of \( A \) with \( H \) as in (7) does not lead necessarily to a conservation law, unless \( A \) is time independent.

Invariant operators are useful to express the dynamics of the state \( \psi(t) \) in terms of superpositions of their eigenvectors with constant coefficients [10]; also to do inverse engineering, as in shortcuts to adiabaticity, so as to find \( H(t) \) from the desired dynamics [11, 12].

\( I(t) \) may be formally defined by (30) for non-Hermitian Hamiltonians too, and its roles to provide a basis for useful state decompositions and inverse engineering are still applicable [11]. Note however that in this context \( I(t) \) is not invariant in an ordinary sense, but rather

\[
\frac{d}{dt}(\hat{\psi}(t)|I(t)\rangle\langle I(t)|\psi(t)) = 0.
\]

The alternative option, yet to be explored for inverse engineering the Hamiltonian, is to consider (linear) operators \( I'(t) \) such that

\[
\frac{\partial I'(t)}{\partial t} - \frac{1}{i\hbar}[H(t), I'(t) - I'(t)H(t)] = 0,
\]

and thus \( \frac{d}{dt}(\psi(t)|I'(t)\rangle\langle I'(t)|\psi(t)) = 0 \).

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[1] Feshbach H. Unified theory of nuclear reactions. Ann. Phys. 1958, 5, 357-390, doi:https://doi.org/10.1016/0003-4916(58)90007-1.
[2] Ruschhaupt, A.; Damborenea, J. A.; Navarro, B.; Muga, J. G.; Hegerfeldt, G. C. Exact and approximate complex potentials for modelling time observables. EPL 2004, 67, 1-7, doi: 10.1209/epl/i2004-10046-4.
[3] Muga, J. G.; Palao, J. P.; Navarro, B.; Egusquiza, I. L. Complex absorbing potentials. Phys. Rep. 2004, 395, 357-428, doi: 10.1016/j.physrep.2004.03.002.
[4] Ruschhaupt, A.; Dowdall, T.; Simón M. A.; Muga, J. G. Asymmetric scattering by non-Hermitian potentials. EPL 2017, 120, 20001, doi: 10.1209/0295-5075/120/20001.
[5] Mostafazadeh A. Pseudo-Hermitian representation of quantum mechanics. Int. J. Geom. Methods Mod. Phys. 2010, 07, 1191, doi:10.1142/S0219887810004816.
[6] Lachezar S. S.; Vitanov, N. V. Dynamical invariants for pseudo-Hermitian Hamiltonians. Phys. Rev. A 2016, 93, 012123, doi: 10.1103/PhysRevA.93.012123.
[7] Wigner, E. P. Group Theory and its application to the quantum mechanics of atomic spectra. Academic Press: New York, USA, 1959; pp. 233-236, ISBN 978-0-1275-0550-3.
[8] Rose, H. E. A course on finite groups. Springer-Verlag: London, UK, 2009, ISBN 978-1-84882-888-9.
[9] Ruschhaupt, A.; Muga, J. G. Atom diode: A laser device for a unidirectional transmission of ground-state atoms. *Phys. Rev. A* **2004** *70*, 061604(R), doi: 10.1103/PhysRevA.70.061604.

[10] Lewis H. R.; Riesenfeld W. B. An Exact Quantum Theory of the Time-Dependent Harmonic Oscillator and of a Charged Particle in a Time-Dependent Electromagnetic Field. *J. Math. Phys.* **1969** *10*, 1458-1473, doi: 10.1063/1.1664991

[11] Ibáñez, S.; Martínez-Garaot, S.; Chen, X.; Torrontegui, E.; Muga, J. G. Shortcuts to adiabaticity for non-Hermitian systems. *Phys. Rev. A* **2011** *84*, 023415, doi: 10.1103/PhysRevA.84.023415.

[12] Torrontegui, E.; Ibáñez, S.; Martínez-Garaot, S.; Modugno, M.; del Campo, A.; Guéry-Odelin, D.; Ruschhaupt, A.; Chen, X.; Muga, J. G. Shortcuts to adiabaticity. *Adv. At. Mol. Opt. Phys.* **2013** *62*, 117-169, doi: 10.1016/B978-0-12-408090-4.00002-5