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# Non-Hermitian Hamiltonians with real eigenvalues coupled to electric fields: from the time-independent to the time dependent quantum mechanical formulation

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We provide a reviewlike introduction into the quantum mechanical formalism related to non-Hermitian Hamiltonian systems with real eigenvalues. Starting with the time-independent framework we explain how to determine an appropriate domain of a non-Hermitian Hamiltonian and pay particular attention to the role played by  $\mathcal{PT}$ -symmetry and pseudo-Hermiticity. We discuss the time-evolution of such systems having in particular the question in mind of how to couple consistently an electric field to pseudo-Hermitian Hamiltonians. We illustrate the general formalism with three explicit examples: i) the generalized Swanson Hamiltonians, which constitute non-Hermitian extensions of anharmonic oscillators, ii) the spiked harmonic oscillator, which exhibits explicit supersymmetry and iii) the  $-x^4$ -potential, which serves as a toy model for the quantum field theoretical  $\phi^4$ -theory.

## I. INTRODUCTION

In general most physicists will almost instinctively associate a non-Hermitian Hamiltonian with unstable states, decaying wavefunctions, resonances and dissipation. Such type of systems have been studied for a long time. They arise for instance when coupling channels in a system in which the wavefunctions factorize into functions which depend on separate sets of variables. The effective Hamiltonians resulting in this manner are non-Hermitian and have *complex* eigenvalues [1]. However, one should note that Hermiticity of the Hamiltonian is only a sufficient condition, which guarantees real eigenvalues and the conservation of probability densities. It needs to be emphasized that it is not a necessary condition and there could be non-Hermitian Hamiltonians with *real* discrete eigenvalue spectra, which then constitute potential candidates for physical applications, such as for instance atomic systems without decay.

Precisely such type of Hamiltonian systems are currently under intense investigation (for a collection of recent results see for instance [2]). The central question in this context is of course how to obtain a consistent quantum mechanical framework. So far much effort has gone into the study of time-independent eigenvalue problems. The main question we wish to address here is how to couple an external time-dependent electric field to a non-Hermitian Hamiltonian with real eigenvalues [3].

Our manuscript is organized as follows: For the benefit of the non-expert and the audience of this conference we commence in section II with a brief reviewlike introduction by recalling some by now well-known facts and arguments on the consistent quantum mechanical formulation of non-Hermitian Hamiltonian systems. In section A we review the time-independent formulation starting with a discussion of how to determine the appropriate domain for a non-Hermitian Hamiltonian from the choice of asymptotic boundary condition. In part 2 of this section we explain the limited role played by  $\mathcal{PT}$ -symmetry. In part 3 of section A we explain how pseudo-Hermiticity can be employed to map almost all relevant problems in

the non-Hermitian scenario to a Hermitian system in the same equivalence class. The two systems obtained in this manner are therefore isospectral. In section B we discuss how this formalism can be extended to include an evolution in time. We describe here gauge transformations, perturbation theory and how to compute various physical quantities in the non-Hermitian setting. In section III we discuss two methods of how to solve one of the key problems in this context, namely how to compute pseudo-Hermitian Hamiltonians. Section IV contains three explicit examples to which the formulation from the previous sections applies: i) the generalized Swanson Hamiltonians, which constitute non-Hermitian extensions of anharmonic oscillators, ii) the spiked harmonic oscillator, which exhibits explicit supersymmetry and iii) the  $-x^4$ -potential, which serves as a toy model for the quantum field theoretical  $\phi^4$ -theory. We state our conclusions and an outlook to further problems in section V.

## II. THE GENERAL FRAMEWORK

### A. Time-independent quantum mechanical formulation

#### 1. The domain of non-Hermitian Hamiltonians

The current interest in this subject was triggered eight years ago [4] by the at the time rather surprising numerical observation that the Hamiltonian

$$H = p^2 - g(iz)^N \quad (1)$$

defined on a suitable domain possesses a real positive and discrete eigenvalue spectrum for integers  $N \geq 2$  with positive real coupling constant  $g$ . This property holds despite it being non-Hermitian  $H \neq H^\dagger$  and unbounded from below, for  $N = 4n$  with  $n \in \mathbb{N}$ . Throughout this paper we use atomic units  $\hbar = e = m_e = c\alpha = 1$ .

Viewing now  $H$  in (1) as a differential operator in position space acting on some wavefunction  $\Phi(z)$ , one needs to specify appropriate boundary conditions in order to

select a meaningful domain. In [4] it was argued that the natural boundary condition,  $\Phi(z) \rightarrow 0$  exponentially for  $|z| \rightarrow \infty$ , requires that one continues the eigenvalue problem into the complex  $z$ -plane. In fact, for  $H$  in (1) it was found that the wedges bounded by the Stokes lines in which this boundary condition holds are given by

$$\mathcal{W}_L(N) = \left\{ \theta \left| -\frac{8+N}{2(N+2)}\pi < \theta < -\frac{4+N}{2(N+2)}\pi \right. \right\}, \quad (2)$$

$$\mathcal{W}_R(N) = \left\{ \theta \left| -\frac{N}{2(N+2)}\pi < \theta < \frac{4-N}{2(N+2)}\pi \right. \right\}, \quad (3)$$

where  $\theta = \arg z$ . To see this one can follow the procedure for an asymptotic expansion of a differential operator as outlined for instance in [5]. Substituting  $\Phi(z) = \exp(\varphi(z))$  into the eigenvalue equation  $H\Phi = \varepsilon\Phi$  yields  $\varphi'' + (\varphi')^2 + g(iz)^N + \varepsilon = 0$ . For  $|z| \rightarrow \infty$  with infinity being an irregular singular point one may assume that  $\varphi'' \ll (\varphi')^2$ . For large  $z$  we can also neglect  $\varepsilon$  in comparison with the potential and obtain

$$\varphi(z) \sim \frac{2\sqrt{g}}{N+2} i^{(1+\frac{N}{2})} z^{(1+\frac{N}{2})} \quad \text{for } |z| \rightarrow \infty. \quad (4)$$

In order to extract the dominating exponential factor in  $\Phi(z)$  and to achieve  $\Phi(z) \rightarrow 0$  for  $|z| \rightarrow \infty$ , we require  $\text{Re } \varphi(z) < 0$ . With  $\theta = \arg z$  this is equivalent to

$$\sin\left(\frac{\pi N}{4} + \frac{2+N}{2}\theta\right) > 0, \quad (5)$$

which amounts to the conditions (2), (3) for the left and the right wedge  $\mathcal{W}_L$  and  $\mathcal{W}_R$ , respectively. Of course (5) allows for many more solutions and therefore possible wedges, but the selection criterion for (2), (3) is to reproduce the conventional wedge for the harmonic oscillator for  $N = 2$ , which is centered around the real axis.

This means the domain of integration, which makes the eigenvalue problem of the non-Hermitian Hamiltonian operator in (1) in position space well defined for the asymptotic boundary condition  $\Phi(z) \rightarrow 0$  exponentially for  $|z| \rightarrow \infty$  is any path in the complex  $z$ -plane which remains inside the wedges  $\mathcal{W}_L$  and  $\mathcal{W}_R$  when it approaches complex infinity. This means any path parameterized as  $z(x)$  with  $x \in \mathbb{R}$ , which satisfies

$$\lim_{x \rightarrow \pm\infty} \arg[z(x)] \in \mathcal{W}_{R/L} \quad (6)$$

guarantees the appropriate boundary condition, namely exponential decay at infinity of the wavefunction  $\Phi(z)$ . For various purposes, for instance when one is concerned about a fast numerical convergence, one can also determine the anti-Stokes lines, that is the domain on which the wavefunction vanishes most rapidly, see e.g. [5]. For  $H$  in (1) the anti-Stokes angles  $\theta_{L/R}^{AS}$  are just in the centre of  $\mathcal{W}_L$  and  $\mathcal{W}_R$  [4].

Permissible domains are therefore usually some form of parameterizations for hyperbolae. For instance a modified version of a parameterization used in [6] was suggested in [7]

$$z_1(x) = x \cos(\theta_R^{AS}) + i \sin(\theta_R^{AS}) \sqrt{a^2 + x^2} \quad (7)$$

with  $a \in \mathbb{R}$ . This clearly satisfied the required asymptotic

$$\lim_{x \rightarrow \pm\infty} \arg[z_1(x)] = \theta_{R/L}^{AS}(N) \in \mathcal{W}_{R/L}(N). \quad (8)$$

for all values of  $N$ . However, as we shall discuss in more detail in section IV certain manipulations depend crucially on the suitable choice of the parameterization and one needs various alternatives. The selection procedure for what is most "appropriate" is largely left to inspired guess work at this stage. As we shall see below, an extremely useful variation of (7) was provided in [8]

$$z_2(x) = -2i\sqrt{1+ix} \quad (9)$$

with

$$\begin{aligned} \lim_{x \rightarrow \infty} \arg[z_2(x)] &= -\frac{\pi}{4} \in \mathcal{W}_R(N) \\ \lim_{x \rightarrow -\infty} \arg[z_2(x)] &= \frac{-3\pi}{4} \in \mathcal{W}_L(N) \end{aligned} \quad (10)$$

for  $N = 3, 4, \dots, 9$ . Another permissible parameterization can be found for instance [9]. We illustrate the above discussion with some examples in figure 1:

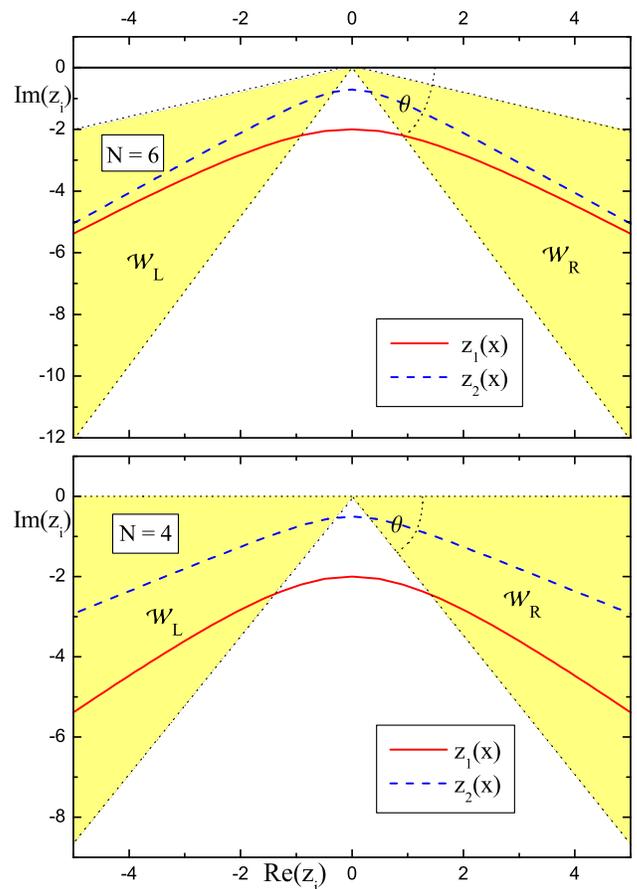


Figure 1: Stoke wedges in which the eigenfunctions of  $H$  in (1) for  $N = 4, 6$  vanish exponentially when  $|z| \rightarrow \infty$ . Permissible paths  $z_1$  with  $a=1$  and  $z_2$  as parameterized in (7) and (9), respectively. The Stokes lines are depicted as dotted lines in the figure.

## 2. $\mathcal{PT}$ -symmetry and real eigenvalues

So how can one explain such unconventional behaviour that a non-Hermitian Hamiltonian possesses a real eigenvalue spectrum? Shortly after the above mentioned observation it was suggested that the reality of the spectrum should be attributed to unbroken  $\mathcal{PT}$ -symmetry [10], that is the validity of the *two* relations

$$[H, \mathcal{PT}] = 0 \quad \text{and} \quad \mathcal{PT}\Phi = \Phi, \quad (11)$$

where  $\Phi$  is a square integrable eigenfunction on some domain of  $H$ . In other words, when the Hamiltonian *and* the wavefunction remain invariant under a simultaneous parity transformation  $\mathcal{P}$  and time reversal  $\mathcal{T}$

$$\begin{aligned} \mathcal{P}: & \quad p \rightarrow -p & \quad z \rightarrow -z \\ \mathcal{T}: & \quad p \rightarrow -p & \quad z \rightarrow z & \quad i \rightarrow -i \\ \mathcal{PT}: & \quad p \rightarrow p & \quad z \rightarrow -z & \quad i \rightarrow -i, \end{aligned} \quad (12)$$

the eigenvalues of  $H$  are real. As an example one sees that obviously the Hamiltonian in equation (1) is  $\mathcal{PT}$ -symmetric. What is less straightforward to see is that for  $N < 2$  the second relation in (11) does not hold. Analytic arguments, which establish these facts for the Hamiltonian (1) may be found in [11, 12].

We shall now outline to what extent  $\mathcal{PT}$ -symmetry can be utilized. Clearly  $\mathcal{P}^2 = \mathcal{T}^2 = (\mathcal{PT})^2 = \mathbb{I}$  and the last relation in (12) implies that the  $\mathcal{PT}$ -operator is an anti-linear operator, i.e. it acts as  $\mathcal{PT}(\lambda\Phi + \mu\Psi) = \lambda^*\mathcal{PT}\Phi + \mu^*\mathcal{PT}\Psi$  with  $\lambda, \mu \in \mathbb{C}$  and  $\Phi, \Psi$  being eigenfunctions of the Hamiltonian  $H$  with eigenenergies  $\varepsilon$ ,  $H\Phi = \varepsilon\Phi$ . The anti-linear nature of the  $\mathcal{PT}$ -operator serves well to establish the reality of the spectrum, i.e.  $\varepsilon = \varepsilon^*$ , when *both* relations in (11) hold. This follows simply from

$$\begin{aligned} \varepsilon\Phi = H\Phi = H\mathcal{PT}\Phi = \mathcal{PT}H\Phi = \mathcal{PT}\varepsilon\Phi = \varepsilon^*\mathcal{PT}\Phi \\ = \varepsilon^*\Phi. \end{aligned} \quad (13)$$

Unfortunately, the anti-linearity is also responsible for the possibility that only the first identity in (11) could hold, but not the second. In this situation one speaks of a broken  $\mathcal{PT}$ -symmetry. The argument leading to this is straightforward [13, 14]: Let us consider first a unitary operator  $U$  for which by definition

$$\langle U\Psi | U\Phi \rangle = \langle \Psi | \Phi \rangle \quad (14)$$

holds for all eigenfunctions  $\Phi, \Psi$  of  $H$ . From equation (14) it follows that  $U\Psi = u\Psi$  with  $|u| = 1$  for all  $\Psi$ , which means that a unitary operator has only one dimensional representations. This property changes for anti-unitary operators  $A$ , as in that case only  $A^2$  is a unitary operator, which can be seen from

$$\langle A^2\Psi | A^2\Phi \rangle = \langle A\Phi | A\Psi \rangle = \langle \Psi | \Phi \rangle. \quad (15)$$

Now we can only deduce from (15) that  $A^2\Psi = a^2\Psi$  with  $|a^2| = 1$  for all  $\Psi$  and this means that an anti-unitary

(which is implied by anti-linearity) operator could have a two dimensional representation  $A\Psi = a^*\Phi$ ,  $A\Phi = a\Psi$ . Indeed when  $a$  is purely imaginary one can not construct a linear combination  $\Omega = \lambda\Phi + \mu\Psi$ , with  $\lambda, \mu \in \mathbb{C}$  of the two so-called flipping states  $\Phi, \Psi$ , which remains invariant under the action of  $A$ . We see that

$$A\Omega = \lambda^*a\Psi + \mu^*a^*\Phi = \lambda\Phi + \mu\Psi \quad (16)$$

implies that  $\mu = \lambda^*a$ ,  $\lambda = \mu^*a^*$  and therefore  $a^2 = 1$ . This means that only for  $a = \pm 1$  the two-dimensional representation is reducible and for purely complex  $a$  it is irreducible. In the latter situation the second relation in (11) does therefore not hold. From (13) we see that  $\mathcal{PT}\Phi$  is an eigenfunction of  $H$  with eigenvalue  $\varepsilon^*$  when  $\Phi$  is an eigenfunction of  $H$  with eigenvalue  $\varepsilon$ . Thus when the second relation in (11) does not hold the eigenvalues of  $H$  come in complex conjugate pairs.

Thus  $\mathcal{PT}$ -symmetry is merely a fairly good guiding principle and serves to identify immediately potentially interesting non-Hermitian Hamiltonian systems. However, as argued above the  $\mathcal{PT}$ -symmetry of  $H$  does not constitute a guarantee for a real eigenvalue spectrum. It remains an open question at this stage to determine under which circumstances the  $\mathcal{PT}$ -symmetry is broken, albeit for Hamiltonians acting in a finite dimensional Hilbert space an algorithm based on stability theory has been provided [15]. In addition one should stress, that  $\mathcal{PT}$ -symmetry can not be regarded as the fundamental property, which explains always the reality of the spectrum for non-Hermitian Hamiltonian systems as there exist also examples with real spectra for which not even the Hamiltonian is  $\mathcal{PT}$ -symmetric [3, 16] (see also examples below). In fact, more fundamental is the necessary and sufficient condition that the Hamiltonian must be Hermitian with regard to *some* positive definite inner product [17] as we shall discuss next.

We summarize the role played by  $\mathcal{PT}$ -symmetry in figure 2:

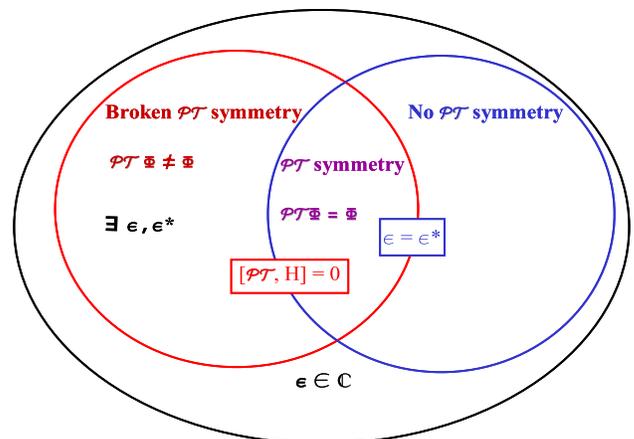


Figure 2:  $\mathcal{PT}$ -symmetry and real eigenvalues

### 3. Pseudo-Hermiticity and real eigenvalues

The formal question of how to establish a consistent quantum mechanical formalism for non-Hermitian Hamiltonian systems has already been discussed in [18] prior to the above mentioned numerical observation. In fact the possibility of extending a Hilbert space by a new intermediate state, which then leads to an indefinite metric has already preoccupied particle physicists more than half a century ago [19]. Some of these old results have recently been re-discovered and developed further. As already mentioned Hermiticity is a useful property as it guarantees the reality of the spectrum. Let us briefly recall this standard argument and discuss how it needs to be altered for the present scenario.

Suppose we have a diagonalizable Hermitian (symmetric) operator  $h$  with regard to the conventional inner product

$$\langle \phi_n | h \phi_m \rangle = \langle h \phi_n | \phi_m \rangle. \quad (17)$$

We use here Hermiticity in the sense that it implies self-adjointness and ignore possible subtleties, which might arise from domain issues. In general we understand here the domain to be the entire real axis. Multiplying next the eigenvalue equations

$$|h\phi_m\rangle = \varepsilon_m |\phi_m\rangle \quad \text{and} \quad \langle h\phi_n| = \varepsilon_n^* \langle \phi_n|. \quad (18)$$

by  $\langle \phi_n|$  and  $|\phi_m\rangle$ , respectively, we obtain

$$\langle \phi_n | h \phi_m \rangle = \varepsilon_m \langle \phi_n | \phi_m \rangle \quad (19)$$

$$\langle h \phi_n | \phi_m \rangle = \varepsilon_n^* \langle \phi_n | \phi_m \rangle. \quad (20)$$

Taking the difference between (19) and (20) thus implies for  $n = m$  that Hermiticity of  $h$  with regard to the standard positive-definite inner product  $\langle \phi_n | \phi_m \rangle$ , i.e. the validity of (17), is a sufficient condition for the energies  $\varepsilon_n$  to be real. Taking next  $n \neq m$  Hermiticity then also implies the orthogonality of the states  $|\phi_n\rangle$  for all  $n$ .

It turns out that for non-Hermitian operators we only need to change the definition for the inner product, i.e. change the metric, to draw the same conclusions [17, 18]. Taking now the domains as discussed in section 3, by definition we obviously no longer have  $\langle \Phi_n | H \Phi_m \rangle = \langle H \Phi_n | \Phi_m \rangle$  for a non-Hermitian operator  $H$  with  $\Phi_n$  obeying the eigenvalue equation

$$H |\Phi_n\rangle = \varepsilon_n |\Phi_n\rangle. \quad (21)$$

Therefore there is no guarantee for the reality of the spectrum and neither for the orthogonality. However, assuming  $\eta$  to be a Hermitian operator with respect to the standard inner product, we can define a new inner product

$$\langle \Phi_n | \Phi_m \rangle_\eta := \langle \Phi_n | \eta^2 \Phi_m \rangle. \quad (22)$$

Supposing now that  $H$  is Hermitian with regard to this new inner product

$$\langle \Phi_n | H \Phi_m \rangle_\eta = \langle H \Phi_n | \Phi_m \rangle_\eta, \quad (23)$$

we may employ exactly the same arguments as above and ensure the reality of the spectrum as well as the orthogonality  $\langle \Phi_n | \Phi_m \rangle_\eta = \delta_{n,m}$ . Note that with regard to the standard inner product one finds in general that  $\langle \Phi_n | \Phi_m \rangle \neq \delta_{n,m}$ , see e.g. [10].

What is left is to characterize in more detail and possibly to determine is the metric operator  $\eta^2$ . Mostafazadeh [17, 20, 21, 22] proposed to assume that  $H$  is a pseudo-Hermitian operator satisfying

$$h = \eta H \eta^{-1} = h^\dagger = \eta^{-1} H^\dagger \eta \Leftrightarrow H^\dagger = \eta^2 H \eta^{-2}, \quad (24)$$

where  $\eta$  is the Hermitian operator with regard to the standard inner product as introduced above. Since the Hermitian Hamiltonian  $h$  and the non-Hermitian Hamiltonian  $H$  are related by a similarity transformation, they belong to the same similarity class and therefore have the same eigenvalues. The corresponding time-independent Schrödinger equations are then simply (18) and (21), where the corresponding wavefunctions are related as

$$\Phi = \eta^{-1} \phi. \quad (25)$$

Having real eigenvalues for the Hermitian Hamiltonian  $h$  then guarantees by construction the same real eigen-spectrum also for  $H$ . In fact the necessary and sufficient condition (23), which ensures the reality of the spectrum for  $H$  follows then from (17)

$$\begin{aligned} \langle \Psi | H \Phi \rangle_\eta &= \langle \Psi | \eta^2 H \Phi \rangle = \langle \eta^{-1} \psi | \eta^2 H \eta^{-1} \phi \rangle \\ &= \langle \psi | \eta H \eta^{-1} \phi \rangle = \langle \psi | h \phi \rangle = \langle h \psi | \phi \rangle = \langle \eta H \eta^{-1} \psi | \phi \rangle \\ &= \langle H \Psi | \eta \phi \rangle = \langle H \Psi | \eta^2 \Phi \rangle = \langle H \Psi | \Phi \rangle_\eta. \end{aligned} \quad (26)$$

Clearly, when  $\eta$  is Hermitian with regard to the standard inner product it is also Hermitian with regard to the  $\eta$ -inner product (22).

A particular example for an  $\eta$ -inner product is the one introduced in [10]

$$\langle \Psi | \Phi \rangle_{\mathcal{CPT}} := (\mathcal{CPT} |\Psi\rangle)^T \cdot |\Phi\rangle, \quad (27)$$

where the new operator  $\mathcal{C}$ , with  $\mathcal{C}^2 = \mathbb{I}$ ,  $[H, \mathcal{C}] = 0$  and  $[\mathcal{C}, \mathcal{PT}] = 0$ , is employed. In position space it reads  $\mathcal{C}(x, y) = \sum_n \Phi_n(x) \Phi_n(y)$ . The operators  $\mathcal{C}$  and  $\eta^2$  are simply related as  $\mathcal{C} = \eta^{-2} \mathcal{P}$ .

In addition one should stress that in fact these inner products can also be derived [23, 24] when starting from a biorthonormal basis, which is quite common to use in the study of non-Hermitian Hamiltonian systems with complex eigenvalues, that is decaying states, see e.g. [25, 26].

Crucial for a proper quantum mechanical framework is of course to clarify the nature of the physical observables. In order to be suitable for a physical interpretation, observables  $\mathcal{O}$  have to be Hermitian operators acting in some physical Hilbert space. From what has been outlined above with regard to the inner products, it is natural to take them to be Hermitian with respect to the new  $\eta$ -inner product

$$\langle \Phi_n | \mathcal{O} \Phi_m \rangle_\eta = \langle \mathcal{O} \Phi_n | \Phi_m \rangle_\eta. \quad (28)$$

This implies immediately that when  $o$  is an observable in the Hermitian system, then

$$\mathcal{O} = \eta^{-1}o\eta \quad \Leftrightarrow \quad \mathcal{O} = \eta^{-2}\mathcal{O}^\dagger\eta^2 \quad (29)$$

is an observable in the non-Hermitian system. This means in turn that the standard position operator  $x$  and the momentum operators  $p$  are in general not observable in the non-Hermitian system, but rather their non-Hermitian counterparts  $X$  and  $P$ , respectively. Clearly  $X$  and  $P$  satisfy the standard canonical commutation relations  $[X, P] = i$  when  $[x, p] = i$ . For Hamiltonians  $h, H$ , which admit a polynomial expansion in  $\{x, p\}$ ,  $\{X, P\}$ , it follows then directly from (24) that

$$H(x, p) = \eta^{-1}h(x, p)\eta = h(X, P), \quad (30)$$

$$h(x, p) = \eta^{-1}H^\dagger(x, p)\eta = H^\dagger(X, P). \quad (31)$$

These relations serve for instance as a consistency check when we start with a given non-Hermitian Hamiltonian and construct its Hermitian counterpart by means of a similarity transformation. Moreover (30) provides a simple way to express the non-Hermitian Hamiltonian in terms of the canonical  $(X, P)$ -variables, which have a physical meaning for that system rather than the  $(x, p)$ -variables, which are in general meaningless in that context. In addition, one may use (30) as a principle to construct non-Hermitian Hamiltonians with real spectra from a given Hermitian Hamiltonian and a set of canonical variables and vice versa with (31). When  $\eta$  is  $\mathcal{PT}$ -symmetric in the  $(x, p)$ -variables the corresponding quantities in the non-Hermitian system will be  $\mathcal{PT}$ -symmetric in the  $(X, P)$ -variables.

We conclude with a final comment in regard to the uniqueness of the metric operator  $\eta^2$ . In fact there are various types of ambiguities arising, which we comment on in section III when we discuss how to compute  $\eta^2$  explicitly. In [18] Scholtz, Geyer and Hahne proved that the metric operator  $\eta^2$  is uniquely determined on a Hilbert space if and only if a set of observables  $\mathcal{O}_i$  with respect to (28) is irreducible on this Hilbert space. The latter means that there is no bounded operator besides the identity, which commutes with all observables  $\mathcal{O}_i$ . Taking this result into account allows to move the nature of the ambiguities from the metric to the specification of the set of observables. As we shall see below a subset or even one observable might be enough in practise.

## B. Time-dependent quantum mechanical formulation

Let us now discuss how to couple a laser field to the non-Hermitian Hamiltonians  $H$ , which have the properties described above. In the simplest scenario, i.e. if the parameters involved lie within a non-relativistic regime and the dipole approximation holds, such a field can be approximated by a time-dependent electric field  $E(t)$ . In the following, we will briefly recall our recent results on

the temporal evolution of the resulting system [3]. For simplicity, we assume that  $E(t)$  is linearly polarized and has a finite duration  $\tau$ .

Within a Hermitian framework and in the length gauge, such an evolution is described by the time-dependent Schrödinger equation

$$i\partial_t\phi(t) = h_l(t)\phi(t), \quad (32)$$

where

$$h_l(t) = \frac{p^2}{2} + V(x) + xE(t) = h + xE(t) \quad (33)$$

is the Stark-LoSurdo Hamiltonian [27, 28]. For a pulse of finite duration,  $h\phi(0) = \varepsilon\phi(0)$  and  $h\phi(\tau) = \varepsilon\phi(\tau)$ . We assume here that  $h$  possesses a non-Hermitian counterpart  $H$  which is in the same equivalence class, i.e. the validity of the first relation in (24).

### 1. Time-evolution operators

The central quantity of interest in this context is the time-evolution operator

$$u(t, t') = T \exp\left(-i \int_{t'}^t dsh(s)\right), \quad (34)$$

which evolves a wavefunction from a time  $t'$  to  $t$ , that is  $\phi(t) = u(t, t')\phi(t')$ . In (34),  $T$  denotes the time ordering. One should note that, in general,  $u(t, t') \neq \exp[-ih(t-t')]$ . In fact, such a relation only holds for Hamiltonians which are not explicitly time-dependent, as is not the case for the scenario we have in mind.

When  $h(s)$  is a self-adjoint operator in some Hilbert space,  $u(t, t')$  satisfies the relations [29, 30, 31]

$$\begin{aligned} i\partial_t u(t, t') &= h(t)u(t, t'), \\ u(t, t')u(t', t'') &= u(t, t'') \text{ and } u(t, t) = \mathbb{I}. \end{aligned} \quad (35)$$

We will now assume that the similarity transformation  $\eta$  extends to the time-dependent case. Thus,  $H(t) = \eta^{-1}h(t)\eta$ , with  $H(t) \neq H^\dagger(t)$ . We take  $\eta$  to be time-independent. This allows us to guarantee that the relations

$$\begin{aligned} i\partial_t U(t, t') &= H(t)U(t, t'), \\ U(t, t')U(t', t'') &= U(t, t'') \text{ and } U(t, t) = \mathbb{I}, \end{aligned} \quad (36)$$

for the time-evolution operator  $U(t, t') = \eta^{-1}u(t, t')\eta$  associated to the non-Hermitian Hamiltonian  $H(t)$ , also hold. Then this operator fulfills the condition  $U^\dagger(t, t') = \eta^2 U^{-1}(t, t')\eta^{-2}$ , which follows from  $u^\dagger(t, t') = u^{-1}(t, t')$ .

It is worth stressing that we make no simplifying assumption on the time dependence of the Hamiltonian. In fact, the only requirements involved in our approach are i) that  $H$  be pseudo-Hermitian and ii) that the similarity transformation  $\eta$  be time-independent. Such conditions

guarantee that the time-dependent Schrödinger equation and the relations involving the time evolution operator remain valid also in the non-Hermitian case.

These conditions, however, are far more general than those normally encountered in the literature. In fact, most studies make several simplifying assumptions on the time-evolution operator, in the sense that they concentrate on Hamiltonians which are either not explicitly time-dependent, or which vary adiabatically and/or periodically with time. The first scenario is addressed by either solving the eigenvalue problem  $H\Phi = \varepsilon\Phi$ , or, at most, by employing the time-evolution operators  $U(t, t') = \exp[-iH(t - t')]$ .

The remaining situations are widespread in the atomic physics literature, in the context of open quantum systems. Roughly speaking, if a system is close to the adiabatic limit this means that it is varying so slowly that the problem can be reduced to solving eigenvalue equations of the form  $H(t)\Phi(t) = \varepsilon_n(t)\Phi(t)$ . In a standard, Hermitian framework, this implies that  $\partial_t u(t)u^\dagger(t) \ll u(t)h(t)u^\dagger(t)$ , and that transitions between different time-dependent eigenstates of  $H(t)$  will be induced by perturbations around the adiabatic limit. Specifically for a system coupled to an external laser field, the time-dependent energies  $\varepsilon_n(t)$  give the field-dressed states (for a first derivation of the adiabatic theorem and for an extension of such a theorem to non-Hermitian open quantum systems, see [32] and [33], respectively). For periodic fields, such a procedure is closely related to the Floquet theory, for which there also exists time-dependent ‘‘quasienergies’’. This approach may be problematic if the field varies abruptly with time, such as, for instance, if it is an ultrashort pulse.

## 2. Time-dependent physical quantities

The time-evolution operators characterized in the previous subsection may then be employed to compute various quantities of physical interest, such as for instance the transition probability

$$\mathcal{P}_{n \leftarrow m} = \left| \langle \Phi_n | U(t, 0) | \Phi_m \rangle_\eta \right|^2 = |\langle \phi_n | u(t, 0) | \phi_m \rangle|^2, \quad (37)$$

from an eigenstate  $|\phi_m\rangle$  to  $|\phi_n\rangle$  of the Hermitian electric field-free Hamiltonian  $h$  or eigenstate  $|\Phi_m\rangle$  to  $|\Phi_n\rangle$  of the non-Hermitian electric field-free Hamiltonian  $H$ . Another physical quantity of interest is the time evolution for the expectation value of an observable in the state  $n$  is

$$\begin{aligned} \mathcal{O}_n(t) &= \langle U(t, 0)\Phi_n(0) | \mathcal{O} U(t, 0)\Phi_n(0) \rangle_\eta \\ &= \langle u(t, 0)\phi_n(0) | \mathcal{O} u(t, 0)\phi_n(0) \rangle_\eta \\ &= o_n(t). \end{aligned} \quad (38)$$

In a similar way we may proceed to compute ionization rates and probabilities etc., but these examples are sufficient to see that, as in the time-independent scenario,

the relevant computations for the non-Hermitian system can be translated into the Hermitian one, provided the  $\eta$ -operator is known.

## 3. Gauge transformations

Apart from employing the length-gauge Hamiltonian  $h_l(t)$ , one may describe a Hermitian Hamiltonian system coupled to an electric field in other gauges. Concrete examples are the velocity gauge, obtained by employing the minimal-coupling prescription  $p \rightarrow p - b(t)$ , or the Kramers-Henneberger gauge, obtained with the shift  $x \rightarrow x - c(t)$  in the field-free Hamiltonian  $h$  as introduced in (33). The corresponding Hamiltonians are given by

$$h_v(t) = \frac{(p - b(t))^2}{2} + V(x) = h(p - b(t)) \quad (39)$$

and

$$h_{KH}(t) = \frac{p^2}{2} + V(x - c(t)) = h(x - c(t)), \quad (40)$$

respectively. In equation (39) and (40),

$$b(t) = \int_0^t ds E(s), \quad c(t) = \int_0^t ds b(s) \quad (41)$$

are the momentum transfer  $b(t)$  from the laser field to the system in question and the classical displacement  $c(t)$  in the system caused by the laser field.

Depending on the problem at hand, the gauge choice may considerably facilitate the computations. For instance, the length gauge is very appropriate for perturbation theory in the electric field, as the field coupling involves only one additional term, or for physical interpretations in the low-frequency regime, since it allows the physical picture of an effective time-dependent potential. The Kramers-Henneberger gauge is most useful in the high-frequency regime, especially if one wishes to exploit the periodicity of the field and perform Floquet expansions. Each formulation can be obtained from the other employing gauge transformations. The Hamiltonians in the length, velocity and Kramers-Henneberger gauge are related by

$$h_l(p, x) - xE(t) = h_v(p + b(t), x) = h_{KH}(p, x + c(t)). \quad (42)$$

We will now perform such transformations for non-Hermitian Hamiltonian systems. First, we will replace the wavefunction  $\phi$  in the time-dependent Schrödinger equation related to the Hamiltonian  $h$  by  $\phi = a(t)^{-1}\phi'$ , with  $a(t)$  being some unitary operator. This yields [29, 30, 31]

$$i\partial_t \phi' = h'(t)\phi' = [a(t)h(t)a(t)^{-1} + i\partial_t a(t)a(t)^{-1}] \phi'. \quad (43)$$

Specifically, the standard transformation from the length to the velocity gauge, and from the velocity to the

Kramers-Henneberger gauge, which are extensively used in strong-field laser physics, are given by,

$$a_{l \rightarrow v}(t) = e^{ib(t)x} \quad \text{and} \quad a_{v \rightarrow KH}(t) = e^{id(t)} e^{-ic(t)p}. \quad (44)$$

respectively. In equation (44), in addition to the momentum transfer and classical displacement, we have also introduced the classical energy transfer  $d(t) = \frac{1}{2} \int_0^t ds b(s)^2$ .

If the system is pseudo-Hermitian, one may employ the relation  $\phi = \eta \Phi$  to obtain the gauge transformation

$$i\partial_t \Phi' = [A(t)H(t)A(t)^{-1} + i\partial_t A(t)A(t)^{-1}] \Phi', \quad (45)$$

where

$$a(t) = \eta A(t)\eta^{-1} \quad \text{and} \quad h(t) = \eta H(t)\eta^{-1}, \quad (46)$$

and the expression in brackets, on the right-hand-side of (45), denotes the gauge-transformed Hamiltonian  $H'(t)$ . The gauge transformations  $A(t)$ , as it should be, guarantee the invariance of the physical observables, when computed using the generalized inner product (22). Now the relations

$$\begin{aligned} H_l(X, P) &= H_v(X, P + b(t)) + XE(t) \\ &= H_{KH}(X + c(t), P) + XE(t), \end{aligned} \quad (47)$$

hold for pseudo-Hermitian Hamiltonians.

#### 4. Perturbation theory

Since, in most realistic situations, the time-dependent Schrödinger equation describing the evolution of a system with a binding potential  $V(x)$  subjected to a time-dependent laser field  $E(t)$  does not possess an analytic solution, it is necessary to resort to perturbation theory. In order to construct a perturbative series in a pseudo-Hermitian framework, we will initially consider a time-dependent Hermitian Hamiltonian  $h(t) = h_0(t) + h_p(t)$ , where  $h_0(t)$  and  $h_p(t)$  are also Hermitian and satisfy the time-dependent Schrödinger equation. Using the Du Hamel formula [29, 30, 31], we can express the time-evolution operator  $u(t, t')$  associated to  $h(t)$  as

$$u(t, t') = u_0(t, t') - i \int_{t'}^t u(t, s) h_p(s) u_0(s, t') ds, \quad (48)$$

where  $u_0(t, t')$  is the time evolution operator with respect to  $h_0(t)$ . Equation (48) can then be solved iteratively to an arbitrary order in  $h_p(t)$ , which will be the perturbation. Roughly speaking if  $h_p(t) \ll h_0(t)$ , the series obtained by such means has a great chance to converge. For instance, for weak laser fields and in the length gauge, a natural choice is to take  $h_p(t) = xE(t)$  and  $h_0(t) = p^2/2 + V$ , whereas in the strong-field regime we take  $h_0(t) = p^2/2 + xE(t)$  as the Gordon-Volkov Hamiltonian and the perturbation is chosen as  $h_p(t) = V$ .

Similarly, for the time evolution operator  $U(t, t')$  related to its pseudo-Hermitian counterpart  $H(t) =$

$H_0(t) + H_p(t)$ , with  $H_0(t) = \eta^{-1} h_0(t) \eta$  and  $H_p(t) = \eta^{-1} h_p(t) \eta$ , we may also write

$$U(t, t') = U_0(t, t') - i \int_{t'}^t U(t, s) H_p(s) U_0(s, t') ds, \quad (49)$$

where  $U_0(t, t')$  is related to the Hamiltonian  $H_0(t)$ , and the perturbative series is obtained by iterating equation (49) up to the desired order.

*a. The weak intensity regime* As argued in the previous subsection one can in general not compute the time-evolution operator exactly and has to resort to perturbation theory instead. We illustrate here briefly how this works more explicitly in the different intensity regimes.

We commence with the weak intensity regime and we will consider first-order perturbation theory with respect to the external laser field amplitude  $E_0$ . Iterating (49) it follows that to this order the time-evolution operator can be approximated by

$$U^{(1)}(t, 0) = U_0(t, 0) - i \int_0^t U_0(t, s) XE(s) U_0(s, 0) ds, \quad (50)$$

where  $U_0(t, 0) = \exp[-iHt]$ . Subsequently the transition probability (37) from a state  $m$  to  $n$  to this order becomes

$$\mathcal{P}_{n \leftarrow m} = \left| \delta_{nm} - i \langle \Phi_n | X \Phi_m \rangle_\eta \int_0^t ds e^{i(\varepsilon_n - \varepsilon_m)s} E(s) \right|^2. \quad (51)$$

Note here the occurrence of the matrix element  $\langle \Phi_n | X \Phi_m \rangle_\eta = \langle \phi_n | x \phi_m \rangle$ , which results from taking the non-Hermitian version of the Stark-LoSurdo Hamiltonian in (33) to be  $H_l(t) = H + XE(t)$ . In case we add  $xE(t)$  instead of  $XE(t)$  the amplitude  $\langle \phi_n | \eta x \eta^{-1} \phi_m \rangle$  would occur. With our examples below we demonstrate that the latter matrix element is very often unphysical.

*b. The strong field regime* Next we will address the opposite scenario, namely the situation in which the laser field is larger, or at least comparable to the atomic binding forces. Such a physical framework has become of interest since the mid-1980's, when intense lasers became feasible, due to the wide range of phenomena and applications existing in this context. Concrete examples are high-order harmonic generation, above-threshold ionization, or laser-induced single and multiple ionization (for reviews we refer to [34, 35, 36]). In this case, it is a common procedure to perturb around the Gordon-Volkov Hamiltonian, which, in a non-Hermitian framework and in the length gauge, is given by  $H_l^{(GV)}(t) = P^2/2 + XE(t)$ . To first order, the time-evolution operator then reads

$$\begin{aligned} U^{(1)}(t, 0) &= U_l^{(GV)}(t, 0) \\ &\quad - i \int_0^t U_l^{(GV)}(t, s) V(X) U_l^{(GV)}(s, 0) ds, \end{aligned} \quad (52)$$

where the Gordon-Volkov time-evolution operator is given by

$$U_l^{(GV)}(t, 0) = A_{KH \rightarrow l}(t) \exp[-iP^2 t/2] A_{KH \rightarrow l}^{-1}(0). \quad (53)$$

The gauge transformation  $A_{KH \rightarrow l}(t)$ , from the Kramers Henneberger to the length gauge, is written as

$$A_{KH \rightarrow l}(t) = \eta^{-1} e^{ic(t)p} e^{id(t)} e^{-ib(t)x} \eta \quad (54)$$

$$= e^{ic(t)P} e^{id(t)} e^{-ib(t)X}. \quad (55)$$

Obviously, one may also define a Gordon-Volkov Hamiltonian in the velocity gauge as  $H_l^{(GV)}(t) = (P - b(t))^2/2$ . In this case, the corresponding time evolution operator is  $U_v^{(GV)}(t, 0) = e^{ib(t)X} U_l^{(GV)}(t, 0) e^{-ib(0)X}$ .

### III. COMPUTING PSEUDO-HERMITIAN HAMILTONIANS

Having discussed the central role played by pseudo-Hermitian Hamiltonians it is vital to have a constructive method to realize them. In other words we wish to compute Hamiltonians  $h = h^\dagger$  and  $H \neq H^\dagger$  belonging to the same equivalence class. This is a well defined problem, but in most cases very difficult to solve. Here we present two different types of methods to achieve this.

#### A. Similarity transformations from operator identities

Supposing that the similarity transformation (24) can be realized using a Hermitian operator of the form  $\eta = \exp(q/2)$ , the second relation in (24) implies by standard Baker-Campbell-Hausdorff commutation relations that

$$\begin{aligned} H^\dagger &= H + [q, H] + \frac{1}{2!} [q, [q, H]] + \frac{1}{3!} [q, [q, [q, H]]] + \dots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} c_q^{(n)}(H). \end{aligned} \quad (56)$$

For convenience we have introduced here a more compact notation for the  $n$ -fold commutator of the operator  $q$  with some arbitrary operator  $\mathcal{O}$  as

$$c_q^{(n)}(\mathcal{O}) := [q, [q, [q, \dots [q, \mathcal{O}] \dots ]]]. \quad (57)$$

Clearly, if for some integer  $n$  the  $n$ -fold commutator  $c_q^{(n)}(H)$  vanishes the conjugation and therefore the similarity transformation can be computed exactly. In order to see this more explicitly we separate next the non-Hermitian Hamiltonian into its real and imaginary part and bring it into the form

$$H = h_0 + ih_1, \quad (58)$$

with  $h_0 = h_0^\dagger$ ,  $h_1 = h_1^\dagger$ . For the case when one has the condition  $c_q^{(\ell+1)}(h_0) = 0$  for some finite integer  $\ell$ , we found in [3] the closed expressions

$$h = h_0 + \sum_{n=1}^{[\frac{\ell}{2}]} \frac{(-1)^n E_n}{4^n (2n)!} c_q^{(2n)}(h_0), \quad (59)$$

$$H = h_0 - \sum_{n=1}^{[\frac{\ell+1}{2}]} \frac{\kappa_{2n-1}}{(2n-1)!} c_q^{(2n-1)}(h_0), \quad (60)$$

which are related according to the first identity in (24). Here  $[x]$  denotes the integer part of a number  $x$ . The  $E_n$  are Euler's numbers

$$E_1 = 1, \quad E_2 = 5, \quad E_3 = 61, \quad E_4 = 1385, \dots \quad (61)$$

and the  $\kappa_{2n-1}$  may be computed from them according to

$$\kappa_n = \frac{1}{2^n} \sum_{m=1}^{[(n+1)/2]} (-1)^{n+m} \binom{n}{2m} E_m. \quad (62)$$

The first examples are

$$\kappa_1 = \frac{1}{2}, \quad \kappa_3 = -\frac{1}{4}, \quad \kappa_5 = \frac{1}{2}, \quad \kappa_7 = -\frac{17}{8}, \dots \quad (63)$$

Depending on how large  $\ell$  becomes the explicit evaluation of sums in (59) and (60) can become rather complicated. In fact, in most cases the series does not terminate and one has to compute the expressions perturbatively. We shall not discuss such cases here and refer instead to the literature [3, 37, 38, 39, 40].

#### B. Similarity transformations from differential equations

Alternatively one can follow a proposal put forward by Scholtz and Geyer [41, 42] and solve (24) by means of Moyal products instead of computing commutators. The central idea is to exploit isomorphic relations between commutator relations and real valued functions multiplied by Moyal products, which correspond to differential equations. We shall demonstrate that this approach is rather practical and allows to compute pairs of isospectral Hamiltonians  $h = h^\dagger$  and  $H \neq H^\dagger$ , when they are of polynomial nature.

We use a slightly different definition for the Moyal product as in [41, 42], since then the resulting differential equations become simpler [39]. Following for instance [43] we define the Moyal product of real valued functions depending on the variables  $x$  and  $p$  as

$$\begin{aligned} f(x, p) \star g(x, p) &= f(x, p) e^{\frac{i}{2} (\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)} g(x, p) = \quad (64) \\ &= \sum_{s=0}^{\infty} \frac{(-i)^s}{s!} \sum_{t=0}^s (-1)^t \binom{s}{t} \partial_x^t \partial_p^{s-t} f(x, p) \partial_x^{s-t} \partial_p^t g(x, p). \end{aligned}$$

One may then use this expression to turn all operator identities into differential equations. In principle this yields differential equations of infinite order, but when  $f(x, p), g(x, p)$  are of polynomial nature the series terminates and the order will be finite. For instance, if we want to compute the commutator  $[\hat{x}, \hat{p}] = i$  we have to evaluate the corresponding Moyal product relation  $x \star p - p \star x = i$ . Here and in some places below we emphasize the operator nature of the quantities involved by dressing them with hats. In order to keep notations simple we do not always make this rigorous distinction, when it is not strictly necessary. Matters become more complicated when the resulting real valued function depends on  $x$  as well as on  $p$ . As for a function the ordering is of course irrelevant we need a prescription of how to turn such a function back into operator valued expressions. Computing for instance

$$[\hat{x}^2, \hat{p}^2] = 4i\hat{p}\hat{x} - 2 \cong x^2 \star p^2 - p^2 \star x^2 = 4ipx, \quad (65)$$

we observe that we obtain the correct operator valued expression for the last equality when we replace  $px \rightarrow (px + xp)/2$ . In general we have to replace each monomial  $p^m x^n$  or  $x^n p^m$  by the totally symmetric polynomial  $S_{m,n}$  in the  $m$  operators  $p$  and  $n$  operators  $x$

$$S_{m,n} = \frac{m!n!}{(m+n)!} \sum_{\pi} p^m x^n. \quad (66)$$

The sum extends over the entire permutation group  $\pi$ . For our purposes we have usually a given non-Hermitian Hamiltonian  $H$  and wish to compute from the second relation in (24) the Hermitian operator  $\eta^2$ . The corresponding differential equation is then simply

$$H^\dagger(x, p) \star \eta^2(x, p) = \eta^2(x, p) \star H(x, p). \quad (67)$$

Subsequently, one may compute also  $\eta(x, p)$  and  $h(x, p)$  in a similar manner.

A comment is due concerning the uniqueness of the solutions. Having solved various differential equations, we naturally expect some ambiguities in the general solutions, which mirror the possibility of different boundary conditions. However, one should emphasize that these ambiguities are not only present when using Moyal products, but are a general feature occurring also when using commutation relations of the type (59) and (60). It is clear that in that context one may only fix the operator  $q$  up to any operator which commutes with the Hermitian part of  $H$ , that is  $h_0$ . This means that, in (59) and (60), the expressions are insensitive to any replacement  $q \rightarrow q + \tilde{q}$  with  $[\tilde{q}, h_0] = 0$ . A further type of ambiguity, which is always present is a multiplication of  $\eta^2$  by operators which commute with  $H$ , i.e. we could re-define  $\eta^2 \rightarrow \eta^2 Q$  for any  $Q$ , which satisfies  $[Q, H] = 0$ .

It should be mentioned that there are also other possibilities to evaluate the similarity transformations, such as for instance suggested in [44] or directly by using properties of differential equations [45].

Let us now demonstrate with some concrete examples how the above mentioned formalism can be applied.

#### IV. (QUASI) EXACTLY SOLVABLE MODELS

Non-Hermitian Hamiltonians may arise for various different reasons. In the following we provide three such examples, which all arise from quite different arguments and thus provide several types of motivations to study non-Hermitian Hamiltonian systems.

##### A. The generalized Swanson Hamiltonian

One type of non-Hermitian Hamiltonian system arises from a purely mathematical consideration simply by perturbing a Hermitian Hamiltonian by adding a non-Hermitian term. We start with a straightforward example, which results when perturbing the anharmonic oscillators

$$h_n^0(\alpha) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^n \quad (68)$$

for  $n = 1, 2, 3, \dots$  and  $\alpha \in \mathbb{R}$ . Defining now the Hermitian operators  $\eta_m = \exp(q_m/2)$  with  $q_m = 2g/mx^m$  for  $m = 1, 2, 3, \dots$  it is straightforward to compute that

$$c_{q_m}^{(1)}(h_n^0(\alpha)) = ig(px^{m-1} + x^{m-1}p) \quad (69)$$

$$c_{q_m}^{(2)}(h_n^0(\alpha)) = -4g^2x^{2m-2} \quad (70)$$

$$c_{q_m}^{(3)}(h_n^0(\alpha)) = 0 \quad (71)$$

for all  $n, m \geq 0$ . With (69)-(71) the generic expressions (59) and (60) yield with  $\ell = 2$

$$h_{n,m}^{GS}(\alpha, g) = h_n^0(\alpha) + \frac{1}{2}g^2x^{2m-2} \quad (72)$$

$$H_{n,m}^{GS}(\alpha, g) = h_n^0(\alpha) - i\frac{g}{2}(px^{m-1} + x^{m-1}p), \quad (73)$$

which are related according to the first relation in (24). In the special case  $n = m = 2$ , the Hamiltonian  $H_{2,2}^{GS}$  becomes the Swanson Hamiltonian discussed in [42, 46, 47] upon some change in the conventions for the coupling constants. This Hamiltonian arises in the second quantization  $H = c_1aa + c_2a^\dagger a^\dagger + c_3a^\dagger a$  where the  $c_i$  are coupling constants and  $a^\dagger = (x - ip)/\sqrt{2}$ ,  $a = (x + ip)/\sqrt{2}$  are the usual creation and annihilation operators, respectively. The sequence of Hamiltonians (73) illustrates our assertion on the limitations of  $\mathcal{PT}$ -symmetry in section II A 1, that there are non-Hermitian Hamiltonians with real energy spectra which are, however, not  $\mathcal{PT}$ -symmetric. As one easily sees  $H_{n,m}^{GS}(\alpha, g)$  is not  $\mathcal{PT}$ -symmetric when  $m$  is odd, but still has a Hermitian counterpart and therefore real eigenvalues.

Let us next assume that we had simply given the non-Hermitian Hamiltonian and we wanted to compute the  $\eta$ -operator. For instance, for  $H_{2,2}^{GS}(\alpha, g)$  and  $H_{4,2}^{GS}(\alpha, g)$  the corresponding equations (67) become

$$0 = 4gpx\eta^2 + 2\alpha x\partial_p\eta^2 - 2p\partial_x\eta^2 + g\partial_p\partial_x\eta^2, \quad (74)$$

$$0 = 4gpx\eta^2 + 4\alpha x^3\partial_p\eta^2 - 2p\partial_x\eta^2 + g\partial_p\partial_x\eta^2 - \alpha x\partial_p^3\eta^2,$$

respectively. Both equations are easily solved by  $\eta^2 = \exp(gx^2)$ , thus confirming our previous calculation.

Having the operator  $\eta = \exp(gx^m/m)$  at hand we compute from (29) the observables which correspond to the position and momentum operator in the non-Hermitian systems  $H_{n,m}^{GS}(\alpha, g)$  as

$$X = x \quad \text{and} \quad P = p - igx^{m-1}, \quad (75)$$

respectively. Then it is easily verified that indeed (30), (31) and (47) hold.

With regard to the uniqueness of this solution one can see that the first equation in (74) is also solved by  $\tilde{\eta}^2 = \exp(-g/\alpha p^2)$ . In fact for what has been remarked at the end of the last section, it is clear that there should be more solutions corresponding to  $\tilde{\eta}^2 = \exp(g\hat{x}^2)f(h_2^0(\alpha))$ , with  $f$  being some arbitrary well behaved function restricted by the demand that  $\Phi = \tilde{\eta}^{-1}\phi$  remains a bounded function. Obviously  $\tilde{\eta}^2 = \tilde{\eta}^2$  for  $f(x) = \exp(-2gx/\alpha)$ . To see that other choices for  $f(x)$  will also lead to solutions of (74) is less straightforward as we have to turn the operator valued expressions for  $\tilde{\eta}^2$  first into real valued functions before we can verify (74).

Let us next illustrate how to fix the ambiguities by an explicit choice of the observables in the non-Hermitian system, which is always possible for what has been said at the end of section II A. Demanding for instance that  $X = x$  should be an observable in the non-Hermitian system, it follows immediately that the only choice for  $f(x)$  is  $f(x) = 1$  and therefore (75) is the corresponding set of canonical variables. In turn we could also choose  $\tilde{P} = p$  to be an observable, which leads to  $\tilde{\eta}^2$  and  $\tilde{X} = x - ig/ap$ . For  $m \neq n$  it is not possible choose  $\tilde{P} = p$  to be an observable as one can not find a function  $f(x)$  such that  $\tilde{\eta}^2$  becomes a function of  $p$  only.

## B. The spiked Harmonic Oscillator

A further interesting example is the spiked harmonic oscillator as it exhibits an explicit supersymmetry [48, 49, 50] and therefore also phenomena like degeneracy of the energy eigenvalues and even level crossings. The Hermitian version of this Hamiltonian is simply

$$h^{SHO}(x, p) = \frac{1}{2}p^2 + \lambda^2 x^2 + \frac{\alpha^2 - 1/4}{x^2}. \quad (76)$$

This example is very instructive as it is exactly solvable. The normalized eigenfunctions are

$$\phi_n^\alpha(x) = (-1)^n \sqrt{\frac{x\lambda^{\alpha+1}\Gamma(n+1)}{\Gamma(\alpha+n+1)}} e^{-\frac{\lambda x^2}{2}} x^\alpha L_n^\alpha(\lambda x^2), \quad (77)$$

where the  $L_n^\alpha(x)$  denote the generalized Laguerre polynomials and the eigenenergies are

$$\varepsilon_n^\alpha = \lambda(4n + 2\alpha + 2). \quad (78)$$

Clearly there is a degeneracy of the energy levels for  $\varepsilon_n^{-\alpha} = \varepsilon_{n-\alpha}^\alpha$ . The standard harmonic oscillator Hamiltonian results from (76) for  $\alpha = \pm 1/2$ . The corresponding wavefunctions are related to (77) as  $\phi_n^{1/2} = i^{2n-1}\phi_{2n+1}^{HO}$ ,  $\phi_n^{-1/2} = (-1)^n\phi_{2n}^{HO}$ . The motivation here to introduce an Hermitian counterpart for this Hamiltonian is that one wishes to regularize the singularity of the potential at  $x = 0$ , see e.g. [50].

With  $\eta = \exp(-\xi p)$  one easily produces the desired shift and with (24) one obtains

$$H^{SHO}(x, p) = \frac{1}{2}p^2 + \lambda^2(x - i\xi)^2 + \frac{a^2 - 1/4}{(x - i\xi)^2}. \quad (79)$$

This is an example for which the Moyal products are not very suitable for the computations as the last term in the potential of (79) is responsible for the fact that the related differential equations are of infinite order.

Nonetheless, commutators are easily evaluated in this case and for instance the canonical variables for the non-Hermitian system are computed in a rather trivial way, resulting to

$$X = x - i\xi \quad \text{and} \quad P = p. \quad (80)$$

Once again we verify (30) and (31) for consistency.

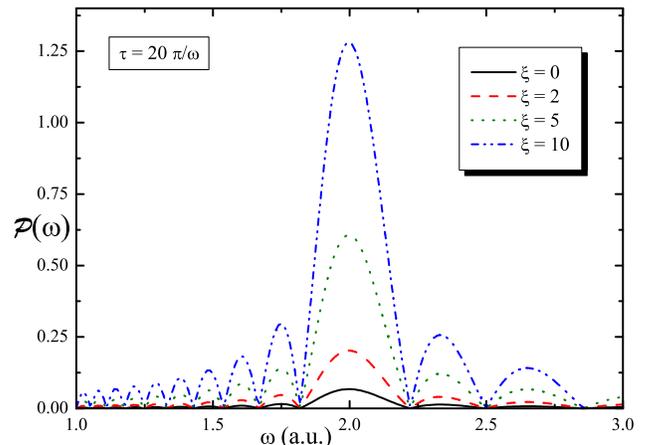


Figure 3: Transition probability for the spiked harmonic oscillator, as functions of the field frequency  $\omega$  and different parameters  $\xi$  introduced in (79). We consider the transition from the energy level  $n = 2$  to  $m = 3$  to first-order perturbation theory with respect to the external laser field. The field amplitude is taken to be weak  $E_0 = 0.005$  a.u. and the coupling constant is chosen as  $\lambda = 0.5$ . The pulse length  $\tau$  and the frequency  $\omega$  are indicated in the figure.

As this example is completely solvable it serves well to illustrate various general features. First we use it to argue that adding  $x E(t)$  instead of  $X E(t)$  to  $H$  in order to construct the non-Hermitian version of the Stark-LoSurdo Hamiltonian is unphysical. To see this we compute the transition amplitude in the weak intensity regime to first order (51), where instead of the amplitude  $\langle \Phi_n | X \Phi_m \rangle_\eta$

we would have  $\langle \phi_n | \eta x \eta^{-1} \phi_m \rangle$ . Now for (80) we would have that  $\langle \phi_n | \eta x \eta^{-1} \phi_m \rangle = \langle \phi_n | x \phi_m \rangle$  for  $n \neq m$ , such that no effect would be visible in the transition amplitude to first order.

Let us therefore take instead the transformation  $\tilde{\eta} = \exp(-\xi p^2)$ . We then compute the canonical variables to

$$\tilde{X} = x - i2\xi p \quad \text{and} \quad \tilde{P} = p. \quad (81)$$

For the corresponding non-Hermitian system  $H(x, p) = h^{SHO}(\tilde{X}, \tilde{P})$  we evaluate next the transition amplitude for  $\phi_2^{0.2} \rightarrow \phi_3^{0.2}$  with  $\lambda = 0.5$ , subjected to a monochromatic linearly polarized electric field  $E(t) = E_0 \sin(\omega t)$  and depict the result in figure 3.

As expected we obtain the main contribution for the transition at  $\varepsilon_3^{0.2} - \varepsilon_2^{0.2} = 2$ . The value  $\xi = 0$  is perfectly reasonable and corresponds to adding  $X E(t)$  to  $H$ , with  $X$  given in (80) for the reasons outlined above. However, for large enough values of  $\xi$  we observe that the transition probability becomes larger than 1, which is of course inconsistent and unphysical. Therefore to add  $x E(t)$  to  $H$  is meaningless in our framework, unless  $x$  can be chosen to be an observable in the non-Hermitian system.

### C. The $-x^4$ potential

A further interesting Hamiltonian arises when we specify in equation (1) the parameter  $N = 4$ , which involves a potential which is unbounded from below. Recently Jones and Mateo [8] established that this Hamiltonian is in fact isospectral to the Hermitian Hamiltonian

$$\tilde{\mathcal{H}} = p^2 + 4g^2 x^4 - 2gx \quad \text{for } x, g \in \mathbb{R} \quad (82)$$

This Hamiltonian is of great interest as it serves as a simplified version for the  $-\phi^4$  quantum field theory, which may for instance be used to mimic the Higgs mechanism. To obtain the Hamiltonian (82) from (1) with  $N = 4$  one needs to pass via two auxiliary Hamiltonians as follows

$$H(z) \xrightarrow{z(x)} H(x) \xrightarrow{\eta} h = h^\dagger \xrightarrow{FT} \tilde{\mathcal{H}}. \quad (83)$$

All manipulation in (83) are spectrum preserving. In the first step the general idea [6] was used to map the contour from within the wedges  $\mathcal{W}_L$  and  $\mathcal{W}_R$  back to the real axis. As discussed in section II A 1 there are many possible parameterization, which guarantee the appropriate boundary condition. Unfortunately, there is no constructive method to select out the most useful contour within the wedges and this choice remains a matter of inspired guess work [8]. Here the best choice is guided by the desire to be able to construct a similarity transformation  $\eta$ , which maps the non-Hermitian Hamiltonian  $H$  adjointly into a Hermitian Hamiltonian  $h$ . Hitherto, this procedure was only successful in an exact manner for the class of Hamiltonians in (1) with  $N = 4$ , in which case  $\eta$  can be constructed exactly either by operator methods [8], differential-equation techniques [45] or Moyal products

[39]. Even for the next example  $N = 6$  the same transformation used as in [8] does not yield an exact similarity transformation [51]. The last step in (83) in the case  $N = 4$  is to transform  $h$  into the Hamiltonian  $\tilde{\mathcal{H}}$  (82) via a Fourier transformation.

Concretely, we exchange now the constant  $g$  by  $\varepsilon$  in (1) with  $N = 4$  and obtain  $H = -d^2/dz^2 - \varepsilon z^4$  thereafter. Using now the parameterization  $z_1(x)$  as defined in (7) one obtains the non-Hermitian Hamiltonian

$$H^{x^4} = \hat{p}^2 - \frac{\hat{p}}{2} + \alpha \hat{x}^2 - \alpha + ig \left( \frac{\{\hat{x}, \hat{p}^2\}}{2} - 2\alpha \hat{x} \right), \quad (84)$$

The domain of  $H^{x^4}$  is now the entire real axis, where  $\alpha = 16\varepsilon$  and the coupling constant  $g$  has been introduced to separate off the non-Hermitian part [8, 39]. Next we want to compute  $\eta$  by means of Moyal products. For this we have to convert  $H$  first into a real valued function and have to substitute the anti-commutator with the Moyal products. Thus we have to replace  $\{\hat{x}, \hat{p}^2\}$  by  $x \star p^2 + p^2 \star x = 2xp^2$ . Subsequently we can use (64) and the differential equation (67) for the Hamiltonian (84) in the unknown quantity  $\eta^2(x, p)$  becomes

$$0 = 4gp^2 x \eta^2 - 8gx\alpha \eta^2 - 4x\alpha \partial_p \eta^2 - \partial_x \eta^2 + 4p \partial_x \eta^2 + 2gp \partial_p \partial_x \eta^2 - gx \partial_x^2 \eta^2. \quad (85)$$

We can solve this by

$$\eta^2 = e^{\frac{gp^3}{3\alpha} - 2gp}, \quad (86)$$

such that  $\eta = e^{\frac{gp^3}{6\alpha} - gp}$ . From (24) we obtain thereafter the Hermitian Hamiltonian

$$h^{x^4} = \hat{p}^2 - \frac{\hat{p}}{2} + \alpha (\hat{x}^2 - 1) + g^2 \frac{(\hat{p}^2 - 2\alpha)^2}{4\alpha}. \quad (87)$$

Let us compare how these expressions are obtained by means of operator identities. In principle we have to make a general ansatz to find  $q$ , but having already found  $\eta$  we can simply extract it from (86)

$$q = \frac{g}{3\alpha} p^3 - 2gp \quad (88)$$

and verify the corresponding expressions. From (84) we find that

$$h_0^{x^4} = \hat{p}^2 - \frac{\hat{p}}{2} + \alpha (\hat{x}^2 - 1). \quad (89)$$

Next we compute the  $n$ -fold commutators

$$c_q^{(1)}(h_0^{x^4}) = 4ig\alpha x - ig\{x, p^2\} \quad (90)$$

$$c_q^{(2)}(h_0^{x^4}) = -g^2 \frac{2}{\alpha} (p^2 - 2\alpha)^2 \quad (91)$$

$$c_q^{(3)}(h_0^{x^4}) = 0. \quad (92)$$

With  $\ell = 2$  we then find that the generic expression (59) for the Hermitian Hamiltonian yields precisely (87) and

the generic expression (60) for the non-Hermitian Hamiltonian gives (84).

Now the non-Hermitian system in terms of its canonical variables

$$X = x + \frac{ig}{2a}(p^2 - 2a) \quad \text{and} \quad P = p, \quad (93)$$

results from  $H^{x^4}(x, p) = h^{x^4}(X, P)$ . In addition we verify  $h^{x^4}(x, p) = (H^{x^4})^\dagger(X, P)$ .

In this case it suffices to choose  $P = p$  as an observable to make the metric unique. Note also that it is not possible to demand  $X = x$  to be an observable as we can not find a function  $f(x)$  such that all functional dependence on  $p$  is eliminated from the term  $q + f(h_0^{x^4})$ .

## V. CONCLUSIONS

Given a non-Hermitian time-independent Hamiltonian  $H$ , we argued that the analogue of the Stark-LoSurdo Hamiltonian should be

$$H_l(t) = H + XE(t), \quad (94)$$

where  $X = \eta^{-1}x\eta$  is the position operator in the non-Hermitian system. As we have shown when we simply add  $xE(t)$  to  $H$ , we obtain unphysical results unless  $x$  is an observable in the non-Hermitian system. However, we also demonstrated that this is not always possible and  $x$  is often degraded to be a mere auxiliary variable in the non-Hermitian system.

As in the time-independent scenario we saw that once the similarity transformation is known, one can easily translate all the relevant calculations into the Hermitian system. The situation is less straightforward when the transformation  $\eta$  and therefore the Hermitian system is not known. In that case one may take our expressions as benchmarks and think of various different approximation schemes, such as standard perturbation theory, a perturbation via the  $\mathcal{C}$ -operator, Floquet type approximations for periodic potentials etc.

From what has been said one may adopt a rather pessimistic standpoint and conclude that in the end the non-Hermitian formulation is in most cases a mere change of metric of a well posed Hermitian problem. Nonetheless, even leaving the technical difficulty aside to establish the precise relation between these conceptually different formulations, it has been successfully argued that the non-

Hermitian formulation is often more natural and simplifies computations [52, 53]. For an atomic physicist this is of course a natural scenario when we compare these alternative formulations with treatments in various gauges, which are also just different ways to express the same physical quantity. It is a well established fact that different choices of gauges often drastically simplify problems in that context and allow for a more intuitive interpretation. For instance, tunneling processes can be visualized and interpreted more easily in the length gauge formulation, since then one may picture the problem in terms of a time-dependent effective potential barrier, whereas all other gauges would obscure this intuitive physical interpretation. Furthermore, phenomena occurring in the context of high frequency fields are most intuitively understood when viewed in a time-dependent dichotomous potential in the Kramers-Henneberger gauge

Let us conclude by commenting on some of the immediate open problems, which follow from what we discussed. Concerning the time-dependent treatment it would be interesting to change the current set-up by allowing  $\eta$  to be time-dependent.

Having entirely focussed on the pseudo-Hermitian nature of the Hamiltonians involved, we want to conclude with a final comment on the role played by  $\mathcal{PT}$ -symmetry in the time-dependent setting. When  $[\mathcal{PT}, \eta] = 0$  the term  $XE(t)$  is only  $\mathcal{PT}$ -symmetric when  $E(-t) = -E(t)$ . This means that  $\mathcal{PT}$ -symmetry depends on the explicit form of the laser pulse. Taking for instance a typical pulse for a laser field with frequency  $\omega$ , amplitude  $E_0$  and Gaussian enveloping function  $f(t)$ , that is of the form  $E(t) = E_0 \sin(\omega t) f(t)$ , the term  $xE(t)$  would be  $\mathcal{PT}$ -invariant. However, the perfectly legitimate replacement  $\sin(\omega t) \rightarrow \cos(\omega t)$  in this field would break the  $\mathcal{PT}$ -invariance. Recall that in this context the electric field is treated classically. For a discussion of  $\mathcal{PT}$ -symmetry for a full quantum electrodynamic setting we may refer to [54, 55]. However, for the physical applications we dealt with in this manuscript,  $\mathcal{PT}$ -invariance is not a relevant issue, since the pulse is always chosen such that  $H\Phi(0) = \varepsilon\Phi(0)$  and  $H\Phi(\tau) = \varepsilon\Phi(\tau)$ . The consequences of  $\mathcal{PT}$ -symmetry on the eigenvalue problem is therefore only important when considering the full time-independent eigenvalue problem (32). To investigate this full solution of (32), the consequences on the non-Hermitian counterpart with its dressed states [32] would be extremely interesting [56].

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