Time evolution of non-Hermitian Hamiltonian systems

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Abstract: We provide time-evolution operators, gauge transformations and a perturbative treatment for non-Hermitian Hamiltonian systems, which are explicitly time-dependent. We determine various new equivalence pairs for Hermitian and non-Hermitian Hamiltonians, which are therefore pseudo-Hermitian and in addition in some cases also invariant under PT-symmetry. In particular, for the harmonic oscillator perturbed by a cubic non-Hermitian term, we evaluate explicitly various transition amplitudes, for the situation when these systems are exposed to a monochromatic linearly polarized electric field.

1. Introduction

To be able to predict the evolution in time for a Hamiltonian system is of central importance to most practical physical problems. For the standard situation, i.e. when the Hamiltonian is Hermitian, there exist well developed frameworks. Having for instance in mind to anticipate the response of an atomic system described by a Hermitian Hamiltonian when it is subjected to an external time-dependent laser field is an intensively studied problem in the weak and recently also in the strong field regime. In the former case Fermi's golden rule is for instance one of the central results, whereas the latter case leads to interesting new phenomena such as high harmonic generation [1], above threshold ionization [2] and stabilization [3, 4, 5], see also [6, 7] for strong field phenomena in general.

Less developed is the situation regarding non-Hermitian Hamiltonians. Depending on the nature of their eigenvalues non-Hermitian Hamiltonian systems can be investigated in various fundamentally different ways. When the corresponding energy eigenvalues are complex one may essentially keep the standard framework and accept the fact that the non-Hermitian nature of the Hamiltonian will lead to decaying states and wavefunctions. Various investigations concentrate on that particular setting [8, 9, 10, 11, 12, 13, 14]. However, more recently it was observed that a large class of non-Hermitian Hamiltonians possess real and positive spectra [15]. For that situation it is natural to demand preservation of probability density, which is not guaranteed even when the Hamiltonian is time-independent.

By now there exists a considerable amount of results regarding this situation for various single particle systems [16, 17, 18, 19, 20] quantum field theories[1] [23, 24, 25] and also integrable many particle systems [26, 27]. So far most effort has gone into the development of a proper quantum mechanical framework for such systems. The main purpose of this paper is to extend these treatments, such that they include a proper description for the time-evolution for non-Hermitian Hamiltonian systems.

Our manuscript is organized as follows: In order to establish our notation and to highlight the key concepts we review in section 2 the main characteristics for a consistent quantum mechanical description involving non-Hermitian Hamiltonians. In section 3 we generalize the scheme to construct time-independent pseudo Hermitian Hamiltonian systems and provide a systematic procedure, which leads to closed formulae involving Euler's numbers for the equivalence pairs of Hermitian and non-Hermitian Hamiltonians, h and H, respectively. Subsequently we employ that scheme to compute various new equivalence pairs in its exact and perturbative form needed afterwards for the time-dependent treatment. In particular, we generalize non-Hermitian perturbations of the harmonic oscillator to anharmonic oscillators with a wider class of perturbations in an exact formulation. Amongst those new non-Hermitian Hamiltonians is a doubly graded generalization of the Swanson Hamiltonian. Perturbatively we also compute Hermitian counterparts for the harmonic oscillator with an additional igx^n-term for generic n, hitherto only studied for specific cases. In particular, for the case $n = 3$ we provide the explicit formula for all wavefunctions up to order g^3, which turn out to be far simpler than their non-Hermitian counterparts. In section 4 we discuss the time evolution for non-Hermitian Hamiltonian systems in various different gauges and investigate a time-dependent perturbation theory. As a particular example we employ the formalism to compute some transition probabilities for the harmonic oscillator perturbed by igx^3 in an external laser field. We state our conclusions in section 5.

2. Quantum Mechanics involving non-Hermitian Hamiltonians

The possibility that non-Hermitian Hamiltonian systems can possess discrete eigenstates with real positive energies has already been indicated by von Neumann and Wigner [28] almost eighty years ago. More recently this type of systems are under more intense scrutiny and nowadays the properties of these so-called BICs (bound states in the continuum) are fairly well understood for many concrete examples [29, 30, 31] together with their biorthonormal eigenstates [32, 33].

Whereas the above type of Hamiltonians only possess single states with these "strange properties" [28], it was observed eight years ago by Bender and Boettcher [15] that Hamiltonians with potential terms $V = x^2(ix)^\nu$ for $\nu \geq 0$ possess an entirely real and positive spectrum. Since that discovery non-Hermitian Hamiltonians, in the sense that $H^\dagger \neq H$, are under intense investigation. Initially the reality of the spectrum was attributed to the PT-symmetry of the Hamiltonian. In fact, when the wavefunctions are simultaneous

[1] In 1+1 dimensional quantum field theories non-Hermitian Hamiltonian systems are known to be meaningful for some time [21, 22].

eigenstates of the Hamiltonian and the PT-operator one can easily argue that the spectrum has to be real [34]. However, despite the fact that $[PT, H] = 0$, this is not always guaranteed as the PT-operator is an anti-linear operator [19]. As a consequence one may also encounter conjugate pairs of eigenvalues for broken PT-symmetry [34]. To determine whether the PT-symmetry is broken or not one may use various techniques to verify this case-by-case [18, 35]. The central problem arising in this context is that inner products of wavefunctions constituting solutions of the time-independent Schrödinger equation involving non-Hermitian Hamiltonians become indefinite, which is due to the fact that the wavefunctions have to be simultaneous eigenfunctions of H and the PT-operator [36]. Bender, Brody and Jones [34] solved this problem consistently by introducing a new type of inner product

$$\langle \Phi |\, \Phi' \rangle_{CPT} := (CPT\,|\Phi\rangle)^T \cdot \big|\Phi'\big\rangle\,, \tag{2.1}$$

which then indeed leads to a positive definite metric, that is $\langle \Phi_n |\, \Phi_m \rangle_{CPT} = \delta_{nm}$ when labelling the energies by increasing values ε_n. This inner product inherits one complication, which is already present when solving the eigenvalue problem, namely that eventually the wavefunctions Φ no longer vanish for $|x| \to \infty$. In that situation one has to integrate within wedges bounded by the Stokes lines in the complex x-plane [15]. A further initial drawback of this formulation was that the C-operator $C(x,y) = \sum_n \Phi_n(x)\Phi_n(y)$ needed to be determined dynamically, which requires in principle the knowledge of all wavefunctions. Meanwhile also alternative methods have been developed to compute C and this is no longer a real obstacle. For instance, noting that C is a symmetry of the Hamiltonian and in addition an involution, one may compute it alternatively by solving the algebraic equations [37]

$$[C, H] = 0, \qquad [C, PT] = 0 \qquad \text{and} \qquad C^2 = \mathbf{1}\ . \tag{2.2}$$

Even before the discovery of [15] and the introduction of the CPT-inner product (2.1) there have been very general considerations addressing the question of how a consistent quantum mechanical framework can be constructed for non-Hermitian Hamiltonian systems [38]. It was understood that quasi-Hermitian (pseudo-Hermitian) systems would lead to positive inner products. Subsequently this was further developed by Mostafazadeh [39, 40, 41, 42], who proposed that instead of considering PT-invariant Hamiltonians one may investigate pseudo-Hermitian Hamiltonians satisfying

$$h = \eta H \eta^{-1} = h^\dagger = \eta^{-1} H^\dagger \eta \qquad \Leftrightarrow \qquad H^\dagger = \eta^2 H \eta^{-2}, \tag{2.3}$$

with $\eta^\dagger = \eta$. 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

$$h\phi = \varepsilon\phi \qquad \text{and} \qquad H\Phi = \varepsilon\Phi, \tag{2.4}$$

where the wavefunctions are related as

$$\Phi = \eta^{-1}\phi. \tag{2.5}$$

Having real eigenvalues for the Hermitian Hamiltonian h then guarantees by construction a positive spectrum also for H. In fact, this formulation is more general than demanding the Hamiltonian to be PT-symmetric, which is only a sufficient, but not a necessary condition for the spectrum to be real for unbroken PT-symmetry of the wavefunctions. In addition the formulation which involves pseudo-Hermitian Hamiltonians is more intuitive as the reality of the spectrum of H is completely evident. Inner products for the wavefunctions Φ related to the non-Hermitian Hamiltonian H may now simply be taken to be

$$\langle \Phi |\, \Phi' \rangle_\eta := \langle \Phi |\, \eta^2 \Phi' \rangle \,, \tag{2.6}$$

where the inner product on the right hand side of (2.6) is the conventional inner product associated to the Hermitian Hamiltonian h. In case the similarity transformation (2.3) holds, the Hamiltionian H is PT-symmetric and when in addition the solution to (2.2) is taken to be $C = \eta^{-2} P$, the CPT-inner product (2.1), the η-inner product (2.6) and the conventional inner product related to the Hermitian Hamiltonian coincide

$$\langle \Phi |\, \Phi' \rangle_{CPT} = \langle \Phi |\, \Phi' \rangle_\eta = \langle \phi |\, \phi' \rangle \,. \tag{2.7}$$

With regard to (2.7) one may wonder why one requires the CPT -inner products when one may in fact use the η-inner products, or even more radically why one needs the non-Hermitian formulations at all when they can always be related to the standard inner products. In fact, these issues are quite controversially discussed at present [43, 44, 45, 46]. With regard to CPT versus pseudo-Hermiticity, our point of view is that despite the limited restrictive power of PT-symmetry, in particular the fact that is does not guarantee a positive spectrum, it is a very good guiding principle to select potentially interesting non-Hermitian Hamiltonians on the classical level, e.g. for many-particle systems [26, 27]. This property can be read off directly from a classical Hamiltonian, whereas even when one has identified such Hamiltonians, a proper analysis requires the construction of the similarity transformation η of the CPT-operator, which is usually not evident a priori. With regard to the inner products, it appears far easier to construct η rather than the CPT-operator. One apparent virtue of the non-Hermitian formulation, using CPT or η-inner products, is that in this way we may relate simple non-Hermitian Hamiltonians to fairly complicated Hermitian Hamiltonians. It is sometimes argued that the computations in the non-Hermitian framework are simpler to perform [45], but this statement has been challenged [46]. Certainly, as we will see below, this feature can not be elevated to a general principle. We will see that even when the non-Hermitian Hamiltonian looks simpler than its Hermitian counterpart, this is not true for the corresponding wavefunctions, which still take on a simpler form in the Hermitian formulation. Furthermore, we find here in addition that the time-dependent non-Hermitian formulation will always be more complicated or at most of equal degree of complexity than the Hermitian one. It appears to us that the best strategy is to make use of both worlds and switch to one or the other formulation depending on the specific problem at hand.

The main purpose of this paper is to investigate how these frameworks may be translated to the situation when the Hamiltonians become genuinely time-dependent.

3. Construction of pseudo Hermitian Hamiltonians

Accepting that a non-Hermitian formulation of quantum mechanics is more straightforward in a pseudo-Hermitian formulation rather than a CPT-scheme, the question with regard to (2.3) then arises of how to construct Hamiltonians h and H belonging to the same equivalence class. Supposing that the similarity transformation can be realized by using an operator of the form $\eta = \exp(q/2)$, the relation (2.3) implies by standard Baker-Campbell-Hausdorff commutation relations that

$$H^\dagger = H + [q, H] + \frac{1}{2!}[q, [q, H]] + \frac{1}{3!}[q, [q, [q, H]]] + \ldots = \sum_{n=0}^{\infty} \frac{1}{n!} c_q^{(n)}(H). \tag{3.1}$$

For convenience we have introduced here a more compact notation for the n-fold commutator of the operator q with some operator x as

$$c_q^{(n)}(x) := [q, [q, [q, \ldots [q, x] \ldots]]]\,. \tag{3.2}$$

Taking now the non-Hermitian Hamiltonian to be of the form $H = h_0 + ih_1$, with $h_0 = h_0^\dagger$, $h_1 = h_1^\dagger$ the relation (3.1) acquires the form

$$i\,[q, h_0] + \frac{i}{2}[q, [q, h_0]] + \frac{i}{3!}[q, [q, [q, h_0]]] + \ldots = 2h_1 + [q, h_1] + \frac{1}{2}[q, [q, h_1]] + \ldots \tag{3.3}$$

In solving this equation one may start from different given quantities. For instance one may solve for h_1 with given h_0, q, see section 3.1, or one may solve for q with given h_0, h_1, see section 3.2. We will not treat the remaining possibility to construct h_0 for given h_1, q. Furthermore, we will also not discuss the interesting possibility to exploit the isomorphism between commutator relations and Moyal products [47, 48]. This relation allows to translate the commutator relation into a differential equation for η, which may be solved subsequently.

3.1 Exact similarity relations

Some simple exact solutions to (3.3) can be found easily in a quite systematic way by searching for vanishing multi-commutators. For instance, if for a given Hermitian Hamiltonian h_0 we can find some q such that its triple commutator with h_0 is vanishing

$$[q, [q, [q, h_0]]] = 0, \tag{3.4}$$

we can define the non-Hermitian part of H as

$$h_1 = \frac{i}{2}[q, h_0]\,, \tag{3.5}$$

such that the relation (3.3) is solved exactly. According to (2.3) the Hermitian counterpart h of the non-Hermitian Hamiltonian H is then computed to

$$h = \eta\left(h_0 - \frac{1}{2}[q, h_0]\right)\eta^{-1} = h_0 - \frac{1}{8}[q, [q, h_0]]\,. \tag{3.6}$$

We can generalize this construction procedure to any vanishing n-fold commutator of q with h_0. Assuming for this that the sum in (3.3) terminates at some stage, i.e. $c_q^{(\ell+1)}(h_0) = 0$, we make the following ansatz for the non-Hermitian part of H

$$h_1 = i \sum_{n=1}^{\ell} \frac{\kappa_n}{n!} c_q^{(n)}(h_0), \tag{3.7}$$

where the constants $\kappa_n \in \mathbb{R}$ are to be determined such that the relation (3.3) is solved exactly. The substitution of (3.7) into (3.3) then yields

$$\sum_{n=1}^{\ell} \frac{1}{n!} c_q^{(n)}(h_0) = \sum_{n=1}^{\ell} 2\frac{\kappa_n}{n!} c_q^{(n)}(h_0) + \sum_{n=1}^{\ell-1} \sum_{m=1}^{\ell} \frac{1}{n!}\frac{\kappa_m}{m!} c_q^{(n+m)}(h_0). \tag{3.8}$$

Reading off the coefficients of equal n-fold commutators from this equation produces a recursive equation for the constants κ_n

$$\kappa_n = \frac{1}{2} - \frac{1}{2} \sum_{m=0}^{n-1} \binom{n}{m} \kappa_m \qquad \text{for } 1 \leq n \leq \ell. \tag{3.9}$$

With $\kappa_0 = 0$, we can solve (3.9) iteratively and find that all coefficients κ_n for even n vanish, whereas the remaining ones become

$$\kappa_1 = \frac{1}{2}, \quad \kappa_3 = -\frac{1}{4}, \quad \kappa_5 = \frac{1}{2}, \quad \kappa_7 = -\frac{17}{8}, \quad \kappa_9 = -\frac{31}{2}, \quad \kappa_{11} = -\frac{691}{4}, \ldots \tag{3.10}$$

Finally we compute from (2.3) the Hermitian counterpart h of H to

$$h = \eta \left(h_0 - \sum_{n=1}^{\ell} \frac{\kappa_n}{n!} c_q^{(n)}(h_0) \right) \eta^{-1} = \sum_{n=0}^{\ell} \frac{\lambda_n}{2^n n!} c_q^{(n)}(h_0), \tag{3.11}$$

where the constants λ_n are related to the κ_n as

$$\lambda_n = 1 - \sum_{m=0}^{n} 2^m \binom{n}{m} \kappa_m. \tag{3.12}$$

Using the above solutions for the κ_n (3.10), we find that only coefficients λ_n with n even are non-vanishing

$$\lambda_0 = 1, \quad \lambda_2 = -1, \quad \lambda_4 = 5, \quad \lambda_6 = -61, \quad \lambda_8 = 1385, \quad \lambda_{10} = -50521, \ldots \tag{3.13}$$

In fact we observe that these constants are very closely related to Euler's numbers E_n as $\lambda_{2n} = (-1)^n E_n$ for $n = 1, 2, 3, \ldots$With this identification we may alternatively solve the equations (3.12) for the constants κ_m, such that they are also expressed in terms of Euler's numbers

$$\kappa_n = \frac{1}{2^n} \sum_{m=1}^{[(n+1)/2]} (-1)^{n+m} \binom{n}{2m} E_m. \tag{3.14}$$

Here $[x]$ denotes the integer part of x.

Thus given some Hamiltonian h_0, which constitutes the Hermitian part of a non-Hermitian Hamiltonian $H = h_0 + ih_1$, together with an operator q satisfying $c_q^{(\ell+1)}(h_0) = 0$ for some finite integer ℓ, the above procedure provides a systematic way to compute pairs of Hamiltonians

$$h = h_0 + \sum_{n=1}^{[\ell/2]} \frac{(-1)^n E_n}{4^n (2n)!} c_q^{(2n)}(h_0) \qquad \text{and} \qquad H = h_0 - \sum_{n=1}^{[(\ell+1)/2]} \frac{\kappa_{2n-1}}{(2n-1)!} c_q^{(2n-1)}(h_0), \quad (3.15)$$

with $h = h^\dagger$ and $H \neq H^\dagger$, which belong to the same similarity class related by the adjoint action of $\eta = \exp(q/2)$ according to (2.3). The closed formulae in (3.15), together with the line of arguments leading to them, appear to be new.

3.2 Perturbative similarity relations

Often one has a different type of starting point as in the previous subsection and would like to construct h for a completely specified non-Hermitian Hamiltonian H, that is for given h_0 and h_1. In that case we have to solve the commutator relation (3.7) for q and some ℓ. Whenever this is not possible in an obvious manner, one can resort to perturbation theory as originally proposed by Bender, Brody and Jones [37] (see also [49]). To develop this one makes a further assumption on the form of the similarity transformation $\eta = \exp(q/2)$, namely

$$q = \sum_{n=1}^{\infty} g^{2n-1} q_{2n-1}. \quad (3.16)$$

One may argue, by demanding PT-invariance [37], that the powers of g have to be odd. Here we want to guarantee pseudo-Hermiticity and therefore present a slightly different argumentation. We assume the following dependences on the coupling constant g

$$\eta(-g) = \eta(g)^{-1}, \qquad h(g) = h(-g) \qquad \text{and} \qquad H^\dagger(g) = H(-g). \quad (3.17)$$

The first equation is obviously satisfied by the ansatz (3.16), whereas the second and third are supported by the examples presented below. Using then (3.17) the pseudo-Hermiticity

$$H^\dagger(g) = \eta(g)^2 H(g) \eta(g)^{-2} \quad (3.18)$$

simply follows from

$$h(g) = \eta(g) H(g) \eta(g)^{-1} = h(-g) = \eta(-g) H(-g) \eta(-g)^{-1} = \eta(g)^{-1} H^\dagger(g) \eta(g). \quad (3.19)$$

Returning to the discussion of perturbation theory, we see that with the ansatz (3.16) the multi-commutator $c_q^{(n)}(h_0)$ will be at least of the order $\mathcal{O}(g^n)$. This means that a precision of order $\mathcal{O}(g^\ell)$ corresponds to $c_q^{(\ell+1)}(h_0) = 0$, such that the above arguments apply and from (3.7) we obtain

$$h_1 = i \sum_{n=1}^{\ell} \frac{\kappa_n}{n!} g^n \sum_{n_1+n_2+\ldots+n_\ell=n} c_{q_1}^{(n_1)} \left(c_{q_2}^{(n_2)} \left(\ldots c_{q_\ell}^{(n_\ell)}(h_0) \right) \right) + \mathcal{O}(g^{\ell+1}). \quad (3.20)$$

Solving these equations order by order yields the set of equations

$$[h_0, q_1] = \frac{2i}{g} h_1, \tag{3.21}$$

$$[h_0, q_3] = \frac{i}{6g} c^{(2)}_{q_1}(h_1), \tag{3.22}$$

$$[h_0, q_5] = \frac{i}{6g}\left[c^{(1)}_{q_1}(c^{(1)}_{q_3}(h_1)) + c^{(1)}_{q_3}(c^{(1)}_{q_1}(h_1)) - \frac{1}{60} c^{(4)}_{q_1}(h_1)\right], \tag{3.23}$$

which can be used to determine the unknown quantities q_i for $1 \leq i \leq \ell$ recursively, as already noted in [37]. Having determined the q_i to the desired order the Hermitian counterpart h to H results from (3.11) to[2]

$$h = \sum_{n=0}^{[\ell/2]} \frac{(-1)^n E_n}{4^n (2n)!} g^{2n} \sum_{n_1+n_2+\ldots+n_\ell=2n} c^{(n_1)}_{q_1}\left(c^{(n_2)}_{q_2}\left(\ldots c^{(n_\ell)}_{q_\ell}(h_0)\right)\right) + \mathcal{O}(g^{\ell+1}). \tag{3.24}$$

We present here now various time-independent Hamiltonians which belong to the same equivalence class and which we discuss below in its time-dependent variant.

3.3 Non-Hermitian Hamiltonians and their Hermitian counterparts

We will consider some non-Hermitian perturbations of the harmonic or anharmonic oscillators depending on a real coupling constant $\alpha \in \mathbb{R}$

$$h^0_n(\alpha) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^n, \tag{3.25}$$

where x and p are operators obeying the standard canonical commutation relation $[x, p] = i$. Throughout this paper we use atomic units $\hbar = e = m_e = c\alpha = 1$. In the last equation α is of course the fine structure constant and not the coupling constant in (3.25).

3.3.1 Anharmonic oscillator perturbed by $i\sum g_p x^p$

We take as a starting point the harmonic oscillator $h_0 = h^0_2(\alpha)$ and $q = \mu p$, where μ is a real constant which needs to be determined. It is then easily checked that the triple commutator $c^{(3)}_q(h_0)$ indeed vanishes. Therefore we evaluate from (3.5)

$$h_1 = \frac{1}{2}\alpha\mu x = gx, \tag{3.26}$$

where we introduced a new coupling constant $g \in \mathbb{R}$ to simplify the notation. The non-Hermitian Hamiltonian is then of the form

$$H(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + igx. \tag{3.27}$$

[2]After completion of this work we were notified by H.F. Jones that he also noted the occurrence of Euler's numbers in front of the multi-commutators of the perturbative expressions (3.21)-(3.23) [50]. Here they are a consequence of our general formulae (3.15).

According to (3.6) we compute next the Hermitian counterpart of $H(\alpha, g)$ to

$$h(\alpha, g) = \eta H(\alpha, g)\eta^{-1} = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + \frac{1}{2}\frac{g^2}{\alpha}. \tag{3.28}$$

with

$$\eta = e^{\frac{g}{\alpha}p}. \tag{3.29}$$

This equivalent system of Hamiltonians (3.27) and (3.28) follow also directly from (3.15) and for $\alpha = g = 1$, they can already be found for instance in [45].

We may now easily generalize this system by taking for the Hermitian part of the Hamiltonian H the Hamiltonian $h_0 = h_n^0(\alpha)$ as starting point. We compute

$$c_{\mu p}^{(m)}(h_n^0(\alpha)) = \begin{cases} (-i\mu)^m \frac{\alpha}{2} \frac{n!}{(n-m)!} x^{n-m} & \text{for} \quad 1 \leq m \leq n \\ 0 & \text{for} \quad m > n \end{cases}, \tag{3.30}$$

and thus we can take here $\ell = n$ as a cut-off condition in order to compute h_1 from (3.7). For $\mu = 2g$ we then find

$$H_n^{AO}(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^n - \frac{i\alpha}{2} \sum_{m=1}^{[(n+1)/2]} (-1)^{2m} \left(\frac{2g}{\alpha}\right)^{2m-1} \binom{n}{2m-1} \kappa_{2m-1} x^{n+1-2m}, \tag{3.31}$$

where the constants κ_m are determined from (3.14) as sums over Euler's numbers. The Hermitian counterpart results from (3.11) or (3.15) to

$$h_n^{AO}(\alpha, g) = \eta H_n^{AO}(\alpha)\eta^{-1} = h_n^0(\alpha) + \frac{\alpha}{2} \sum_{m=1}^{[n/2]} \left(\frac{2g}{\alpha}\right)^{2m} E_m \binom{n}{2m} x^{n-2m}. \tag{3.32}$$

Clearly, since $c_{p^k}^{(m)}(h_n^0(\alpha)) = 0$ for some finite values of k, n, m, we can generalize this and take $q = \sum_{m=1}^{k} \mu_m p^m$ to construct further conjugate pairs of Hamiltonians. Notice that the dependence of $h_n^{AO}(\alpha, g)$, $H_n^{AO}(\alpha, g)$ and $\eta(g)$ on the coupling constant g respects the aforementioned identities (3.17).

3.3.2 Generalizations of the Swanson Hamiltonian

Next we start again with $h_0 = h_n^0(\alpha)$, but change the operator q in the similarity transformation to $q_m = \mu_m x^m$. It is easy to observe that in this case $c_{\mu_m x^m}^{(3)}(h_n^0(\alpha)) = 0$ for all $m, n \geq 0$. Therefore when taking $\mu_m = 2g/m$ relation (3.5) yields

$$H_{n,m}^S(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^n - i\frac{g}{2}(px^{m-1} + x^{m-1}p), \tag{3.33}$$

and consequently (3.6) gives

$$h_{n,m}^S(\alpha, g) = h_n^0(\alpha) - \frac{1}{8}\left[q_m, \left[q_m, h_n^0(\alpha)\right]\right] = \eta H_{n,m}^S(\alpha)\eta^{-1} \tag{3.34}$$

$$= \frac{1}{2}p^2 + \frac{\alpha}{2}x^n + \frac{1}{2}g^2 x^{2m-2}. \tag{3.35}$$

Notice that when specializing to $n = m = 2$, we obtain the harmonic oscillator

$$h^S_{2,2}(\alpha, g) = h^0_2(\alpha + g^2) \tag{3.36}$$

and $H^S_{2,2}$ becomes the Swanson Hamiltonian [51, 44]

$$H(\alpha, g) = h^0_2(\alpha) - i\frac{g}{2}(xp + px), \tag{3.37}$$

upon changing the conventions for the coupling constants. We further note that only for m odd $ih^1_{n,m}(\alpha)$ is PT-symmetric, which sustains our previous assertion that the requirement of pseudo-Hermiticity covers a larger class of Hamiltonians, which have a positive spectrum. Once more we note that the dependence of $h^S_{n,m}(\alpha, g)$, $H^S_{n,m}(\alpha, g)$ and $\eta(g)$ on the coupling constant g respects the identities (3.17). Notice that if the wave function ϕ is vanishing at $\pm\infty$ this is no longer the case for Φ for odd m.

3.3.3 Harmonic oscillator perturbed by igx^n

In the examples discussed so far we were always able to construct explicitly the similarity transformation η. However, when we start with a given non-Hermitian Hamiltonian this is not always possible. For instance, considering the simplest non-Hermitian perturbation of the harmonic oscillator by $h_1 = gx^3$ [37, 44, 49] and their generalizations

$$H^{HO}_n(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + igx^n \tag{3.38}$$

one has to resort at present to perturbation theory in order to construct η. We adopt now the notation $S_{m,n}$ from [52, 37, 44] for the totally symmetric polynomial in the m operators p and n operators x

$$S_{m,n} = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}x^k p^m x^{n-k} = \binom{m+n}{n}^{-1}\sum_{\pi} p^m x^n. \tag{3.39}$$

In the last expression we take the sum over the entire permutation group π. Since the variables x and p are non-commutative this sum produces $(m+n)!/m!/n!$ non-equivalent terms. The first sum is the much simpler Weyl ordered version of this polynomial. Taking now in (3.21) the harmonic oscillator $h^0_2(\alpha)$ and $h^{(n)}_1 = gx^n$ as our starting point we solve (3.21) for $q^{(n)}_1$ and compute to first order in perturbation theory

$$q^{(3)}_1 = \frac{2}{\alpha}\left(S_{1,2} + \frac{2}{3\alpha}S_{3,0}\right), \tag{3.40}$$

$$q^{(5)}_1 = \frac{2}{\alpha}\left(S_{1,4} + \frac{4}{3\alpha}S_{3,2} + \frac{8}{15\alpha^2}S_{5,0}\right), \tag{3.41}$$

$$q^{(7)}_1 = \frac{2}{\alpha}\left(S_{1,6} + \frac{6}{3\alpha}S_{3,4} + \frac{24}{15\alpha^2}S_{5,2} + \frac{16}{35\alpha^3}S_{7,0}\right), \tag{3.42}$$

$$q^{(9)}_1 = \frac{2}{\alpha}\left(S_{1,8} + \frac{8}{3\alpha}S_{3,6} + \frac{48}{15\alpha^2}S_{5,4} + \frac{64}{35\alpha^3}S_{7,2} + \frac{128}{315\alpha^4}S_{9,0}\right), \tag{3.43}$$

$$\vdots$$

$$q^{(n)}_1 = -\sqrt{\pi}\sum_{k=1}^{[(n+1)/2]}\frac{1}{(-\alpha)^k}\frac{\Gamma\left(k - \frac{1}{2} - \frac{n}{2}\right)}{\Gamma\left(k + \frac{1}{2}\right)\Gamma\left(\frac{1}{2} - \frac{n}{2}\right)}S_{2k-1,n+1-2k}. \tag{3.44}$$

We extrapolated here to the closed formula for all values of n, which we have verified up to $n = 20$. The expression for $q_1^{(3)}$ agrees with the solution found in [37]. The remaining $q_1^{(n)}$ for $n \geq 3$ do not seem to be known in the literature. It is straightforward, but labourous to continue the analysis to higher orders. To next order we compute

$$q_3^{(3)} = 4\left(\frac{32}{15\alpha^5}S_{5,0} + \frac{10}{3\alpha^4}S_{3,2} + \frac{2}{\alpha^3}S_{1,4} - \frac{3}{\alpha^4}S_{1,0}\right), \tag{3.45}$$

The expression for $q_3^{(3)}$ agrees precisely with the one found in [37, 44]. Once again the expressions for higher values of n for $q_3^{(n)}$ seem to be unknown. From (3.15) we then compute the Hermitian counterpart to (3.38) as

$$h_n^{HO}(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 - i\frac{g^2}{4}[x^n, q_1^{(n)}] + \mathcal{O}(g^4). \tag{3.46}$$

The only commutator one needs to evaluate this is [52]

$$[x^n, S_{r,s}] = i\sum_{k=0}^{\lambda(n,r)} \frac{1}{(-4)^k}\frac{1}{(2k+1)!}\frac{n!}{(n-2k+1)!}\frac{r!}{(r-2k+1)!}S_{r-2k-1,s+n-2k-1}, \tag{3.47}$$

where the upper limit of the sum is $\lambda(n,r) = \min([(n+1)/2], [(r+1)/2])$. We then obtain

$$h_n^{HO}(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + \frac{g^2}{2}\sum_{k=1}^{[(n+1)/2]}\sum_{p=0}^{k} c_n^{kp} S_{2(k-p-1),2(n-p-k)} \tag{3.48}$$

with constants

$$c_n^{kp} = (-1)^{k+p+1}\frac{\sqrt{\pi}}{2}\frac{1}{\alpha^k 4^p}\frac{\Gamma(2k)\Gamma(n+1)\Gamma\left(k-\frac{1}{2}-\frac{n}{2}\right)}{\Gamma\left(k+\frac{1}{2}\right)\Gamma\left(\frac{1}{2}-\frac{n}{2}\right)\Gamma(2k-2p-1)\Gamma(n-2p)\Gamma(2p+2)} \tag{3.49}$$

In particular, this reduces to

$$h_3^{HO}(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + \frac{3}{2}\frac{g^2}{\alpha^2}\left(2S_{2,2} + \alpha S_{0,4} - \frac{1}{3}\right) \tag{3.50}$$

$$h_5^{HO}(\alpha, g) = \frac{1}{2}p^2 + \frac{\alpha}{2}x^2 + \frac{5}{2}\frac{g^2}{\alpha^3}\left(\frac{4}{5} + \alpha^2 S_{0,8} - 4\alpha S_{0,4} + 4\alpha S_{2,6} - 16S_{2,2} + \frac{8}{3}S_{4,4}\right) \tag{3.51}$$

The expression for $h_3^{HO}(\alpha, g)$ recovers the one found already in [37, 44]. This equivalence system has been studied extensively and here we shall elaborate further on it taking it as our prime example in the next section. Specifying now $\alpha = 1$ the eigenvalue problem for the non-Hermitian counterpart of $h_3^{HO}(1, g)$, namely $H_3^{HO}(1, g)$ was solved in [53] up to order g^4. The energy eigenvalues were found to be

$$\varepsilon_n = n + \frac{1}{2} + \frac{g^2}{8}(30n^2 + 30n + 11) + \mathcal{O}(g^4). \tag{3.52}$$

The quite lengthy expression for corresponding wavefunctions $\Phi_n(x)$ may be found in [53], see formulae (3.2), (3.3) and (3.6) therein. In the next section we would like to use the

wavefunction for the Hermitian Hamiltonian $h_3^{HO}(1,g)$ instead, which we can simply compute from (2.5). With the help of the explicit expression for $q_1^{(3)}$ we may express the η as a differential operator in x-space

$$\eta = 1 + ig\left(\frac{2}{3}\partial_x^3 - x\partial_x x\right) - g^2\left(x^2 + 2x^3\partial_x - 3\partial_x^2 + \frac{x^4}{2}\partial_x^2 - \frac{8}{3}x\partial_x^3 - \frac{2}{3}x^2\partial_x^4 + \frac{2}{9}\partial_x^6\right). \tag{3.53}$$

A somewhat lengthy but straightforward computation then yields

$$\phi_n(x) = \eta\Phi_n(x) = \frac{i^n e^{-x^2/2}}{\sqrt{\sqrt{\pi}2^n n!}}\left[H_n(x) - g^2 P_n(x) + \mathcal{O}(g^4)\right], \tag{3.54}$$

where the $H_n(x)$ are the n^{th} Hermite polynomials,

$$P_n(x) = \frac{3}{16}\left(2\hat{H}_{n-4}(x) - (8n-4)\hat{H}_{n-2}(x) + (2n+3)H_{n+2}(x) - \frac{1}{8}H_{n+4}(x)\right) \tag{3.55}$$

and $\hat{H}_{n-p}(x) = n(n-1)(n-2)\ldots(n-p+1)H_{n-p}(x)$. The $\phi_n(x)$ are orthonormal wavefunction, which solve the Schrödinger equation up to order g^4. We observe that despite the fact that the Hermitian Hamiltonian h_3^{HO} is more complicated than its non-Hermitian counterpart H_3^{HO}, this is no longer true for their corresponding wavefunctions as $\phi_n(x)$ takes on a much simpler form than $\Phi_n(x)$.

4. Time evolution for non-Hermitian Hamiltonians

Next we consider genuinely time-dependent Hamiltonians. There have been some previous investigations in this direction [8, 9, 10, 11, 12, 13, 14], which, however, do not make use of pseudo-Hermiticity. In addition, in many of these studies the precise meaning of the physical set up remains unclear. For instance, in [10], no explanation is given about the meaning of making the mass time-dependent etc. Here we wish to address a more clear cut physical problem, namely one of the classical questions concerning the behaviour of a quantum mechanical system coupled to an external electromagnetic field. In particular, we have in mind an atom in a time-dependent linearly polarized electric field $E(t)$ in the dipole approximation of finite duration τ. In the length gauge, see section 4.2 for more discussions, this scenario is described by the Stark Hamiltonian and the time-dependent Schrödinger equation reads

$$i\partial_t\phi(t) = \left[\frac{p^2}{2} + V + xE(t)\right]\phi(t) = \left[h + xE(t)\right]\phi(t) = h_l(t)\phi(t), \tag{4.1}$$

We follow here largely the notation of [54, 5, 55]. As the field is taken to be a pulse of finite duration we have $h\phi(0) = E\phi(0)$ and $h\phi(\tau) = E\phi(\tau)$. With regard to our previous discussion we assume now that h has a non-Hermitian counterpart H which is in the same equivalence class, such that $H = \eta^{-1}h\eta$. Hence this involves a potential for which we no longer demand that it is Hermitian, i.e. we allow $V^\dagger \neq V$. Consequently also the resulting Stark Hamiltonian is non-Hermitian $H_l(t) \neq H_l^\dagger(t)$.

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

$$u(t,t') = T\exp\left(-i\int_{t'}^{t} dsh(s)\right), \tag{4.2}$$

which evolves a wavefunction from a time t' to t, that is $\phi(t) = u(t,t')\phi(t')$. T denotes the time ordering. When $h(s)$ is a self-adjoint operator in some Hilbert space, $u(t,t')$ satisfies the relations

$$i\partial_t u(t,t') = h(t)u(t,t'), \qquad u(t,t')u(t',t'') = u(t,t'') \quad \text{and} \quad u(t,t) = \mathbb{I}\,. \tag{4.3}$$

Taking instead a Hamiltonian $H(t)$ which is not self-adjoint and therefore its matrix representation is non-Hermitian these relations no longer hold. However, as we now demonstrate when $H(t)$ is pseudo-Hermitian there is a simple modification of them. Acting adjointly with the time-independent operator η^{-1}on (4.3) and assuming that the similarity transformation $h = \eta H \eta^{-1}$ extends from the time-independent to the time-dependent system

$$h(t) = \eta H(t)\eta^{-1}, \tag{4.4}$$

simply yields

$$i\partial_t U(t,t') = H(t)U(t,t'), \qquad U(t,t')U(t',t'') = U(t,t'') \quad \text{and} \quad U(t,t) = \mathbb{I}\,, \tag{4.5}$$

where we introduced the new time evolution operator $U(t,t')$ associated to the non-Hermitian Hamiltonian $H(t)$ as

$$U(t,t') = \eta^{-1}u(t,t')\eta. \tag{4.6}$$

This time-evolution operator is quasi-pseudo-Hermitian

$$U^\dagger(t,t') = \eta^2 U^{-1}(t,t')\eta^{-2}, \tag{4.7}$$

which follows directly from $u^\dagger(t,t') = u^{-1}(t,t')$. The non-Hermitian counterpart H to the Hermitian Hamiltonian $h_l(t)$ as defined in (4.1) results therefore to

$$H_l(t) = H + \eta^{-1}xE(t)\eta. \tag{4.8}$$

The central assumption is here the validity of the similarity transformation (4.4), which makes the formalism for the treatment of the non-Hermitian problem fairly straightforward. Of course we could also try to solve the problem for the situation when the electric field is coupled directly to the non-Hermitian Hamiltonian H, that means we take it to be of the form

$$\hat{H}_l(t) = H + xE(t). \tag{4.9}$$

In some special cases, namely when $\eta^{-1}xE(t)\eta = xE(t)$, this version is equivalent to (4.8), but in general we require a new kind of formalism for this type of situation as we have now lost the equivalence relation (4.4).

4.1 Equivalent time-dependent pairs of Hamiltonians

Let us illustrate the above for the concrete examples discussed in section 3.

The simplest example is the generalized time-dependent Swanson Hamiltonian, which in the length gauge is simply of the form

$$H^{S,l}_{n,m}(\alpha,g,t) = H^{S}_{n,m}(\alpha,g) + xE(t). \tag{4.10}$$

In this case the formulations (4.8) and (4.9) coincide as $\eta^{-1}xE(t)\eta = xE(t)$. Its time-dependent Hermitian counterpart is therefore simply given by

$$h^{S,l}_{n,m}(\alpha,g,t) = h^{S}_{n,m}(\alpha,g) + xE(t). \tag{4.11}$$

Thus for the Swanson Hamiltonian one obtains the same result whether one couples the electric field to h or H.

For the perturbed anharmonic oscillators, this relation does no longer hold, since the similarity transformation (3.29) does not commute with x, but instead induced a complex shift in $x \to x+ig/2$. From (4.8) the time-dependent versions of the anharmonic oscillators result to

$$H^{AO,l}_{n}(\alpha,g,t) = H^{AO}_{n}(\alpha,g) + xE(t) + igE(t)/2, \tag{4.12}$$

which due to the last term is evidently different from the version (4.9). The time-dependent version of its Hermitian counterpart (3.32) is

$$h^{AO}_{n}(\alpha,g,t) = h^{AO}_{n}(\alpha,g) + xE(t), \tag{4.13}$$

and one has now entirely different systems when coupling the electric field to h or H.

The expressions become more complicated when we have non-trivial commutators between x and η, as for the perturbed harmonic oscillator $H^{HO}_n(\alpha,g)$, for which we only know the similarity transformation perturbatively. In that case the time dependent version becomes

$$H^{HO}_{n}(\alpha,g,t) = H^{HO}_{n}(\alpha,g) + E(t)\sum_{n=0}^{\infty}\frac{(-1)^n}{n!2^n}c^{(n)}_q(x) \tag{4.14}$$

and we have to terminate the infinite sum according to the desired order of precision in powers of g. Using the commutator $[x, S_{m,n}] = imS_{m-1,n}$, which results as a special case of the commutator (3.47), the first order in g is easily computed with the generic expression for $q^{(1)}_n$, see (3.44), to

$$H^{HO}_{n}(\alpha,g,t) = H^{HO}_{n}(\alpha,g) + E(t)\left[x - ig\sum_{k=1}^{[(n+1)/2]}\frac{\sqrt{\pi}}{(-\alpha)^k}\frac{\Gamma\left(k-\frac{1}{2}-\frac{n}{2}\right)}{\Gamma\left(k-\frac{1}{2}\right)\Gamma\left(\frac{1}{2}-\frac{n}{2}\right)}S_{2k-2,n+1-2k}\right]. \tag{4.15}$$

In particular we have

$$H^{HO}_{3}(\alpha,g,t) = H^{HO}_{3}(\alpha,g) + xE(t) + i\frac{g}{\alpha}E(t)\left(x^2 + \frac{2}{\alpha}p^2\right), \tag{4.16}$$

$$H^{HO}_{5}(\alpha,g,t) = H^{HO}_{5}(\alpha,g) + xE(t) + i\frac{g}{\alpha}E(t)\left(x^4 + \frac{4}{\alpha}S_{2,2} + \frac{8}{3\alpha^2}p^4\right). \tag{4.17}$$

The next order is more challenging as it involves commutators between different types of symmetric polynomials $S_{m,n}$ and $S_{r,s}$ for which an expression can be found, however, in [52]

$$[S_{m,n}, S_{r,s}] = in!r! \sum_{k=0}^{\lambda(n-2,r-2)} \frac{{}_3F_2(-1-2k,-m,-s;n-2k,r-2k;1)}{\Gamma(n-2k)\,\Gamma(r-2k)\,\Gamma(2k+2)} S_{m+r-2k-1,n+s-2k-1}, \tag{4.18}$$

where ${}_3F_2$ is a hypergeometric function. We will not present such calculations here.

At this point one may wonder about the PT-symmetry of the non-Hermitian Hamiltonians involved. For instance the term $igE(t)/2$ is only PT-symmetric if $E(-t) = -E(t)$, which means that it depends on the explicit form of the laser pulse. Taking for instance a typical pulse for a laser field with frequency ω, amplitude E_0 and Gaussian enveloping function $f(t)$, that is of the form $E(t) = E_0 \sin(\omega t) f(t)$, would result in a PT-invariant Hamiltonian. However, the perfectly legitimate replacement $\sin(\omega t)$ by $\cos(\omega t)$ would break the PT-invariance. Recall that in this context the electric field is treated classically. A discussion of PT-invariance for a full quantum electrodynamic setting may be found in [56, 57]. For the physical application in mind, PT-invariance is, however, not a relevant issue here, since the pulse is always chosen such that $h\Phi(0) = E\Phi(0)$ and $h\Phi(\tau) = E\Phi(\tau)$ and the eigenvalue problem is therefore only important in the time-independent case. We treat the full solution of (4.1), the consequences on the non-Hermitian counterpart and dressed states [58] elsewhere [59].

4.2 Gauge transformations for non-Hermitian Hamiltonian systems

For various applications it is extremely useful to transform the system to a different gauge. For instance, when having weak fields the length gauge is suitable as it usually involves the electric field just as an additional term, which is very useful for perturbation theory. The Kramers-Henneberger gauge is most useful when one wishes to exploit the periodicity of the field in Floquet analysis, especially for high frequencies. We now want to demonstrate how gauge transformations may be used for non-Hermitian Hamiltonian systems. Replacing for this purpose the wavefunction ϕ in the time-dependent Schrödinger equation related to some Hermitian Hamiltonian h by $\phi = a(t)^{-1}\phi'$, with $a(t)$ being some unitary operator, one obtains the well known identity, see e.g. [54, 5, 55]

$$i\partial_t \phi' = h'(t)\phi' = \left[a(t)h(t)a(t)^{-1} + i\partial_t a(t) a(t)^{-1}\right]\phi'. \tag{4.19}$$

Due to the relation $\phi = \eta\Phi$ it is straightforward to see that the gauge transformation for the non-Hermitian system results to

$$i\partial_t \Phi' = H'(t)\Phi' = \left[A(t)H(t)A(t)^{-1} + i\partial_t A(t) A(t)^{-1}\right]\Phi', \tag{4.20}$$

where the similarity transformation (4.4) extends to the gauge fields as well as to the gauge transformed time-dependent Hamiltonians

$$a(t) = \eta A(t) \eta^{-1} \qquad \text{and} \qquad h(t) = \eta H(t) \eta^{-1}. \tag{4.21}$$

Note that the gauge transformations $A(t)$ guarantee that physical observables remain invariant, when computed using the generalized inner product (2.6).

In the context of laser-matter interaction, there are standard gauge transformations, from the length to the velocity gauge and from the velocity to the Kramers-Henneberger gauge

$$a_{l\to v}(t) = e^{ib(t)x} \qquad \text{and} \qquad a_{v\to KH}(t) = e^{id(t)}e^{-ic(t)p}, \tag{4.22}$$

respectively, involving the classical momentum transfer $b(t)$, the classical displacement $c(t)$ and the classical energy transfer $d(t)$, from the laser field to the system in question. Such quantities are defined as

$$b(t) = \int_0^t dsE(s), \qquad c(t) = \int_0^t dsb(s) \quad \text{and} \quad d(t) = \frac{1}{2}\int_0^t dsb(s)^2. \tag{4.23}$$

In the Hermitian case, the Hamiltonians in the length, velocity and Kramers-Henneberger gauge are related as

$$h_l(p,x) - xE(t) = h_v(p+b(t),x) = h_{KH}(p,x+c(t)). \tag{4.24}$$

Physically, in the length gauge, the coupling with the field can be understood as a laser-induced dipole moment. In the velocity gauge, such a coupling appears as a shift $p \to p-b(t)$ in the canonical momentum, corresponding to the well-known minimal coupling procedure. Finally, in the Kramers-Henneberger gauge, there is a displacement $x \to x - c(t)$ in the coordinate x, which can be interpreted as time-dependent binding potential [60]. For their pseudo-Hermitian counterparts H, one has in general

$$H_l(p,x) - \eta^{-1}xE(t)\eta \neq H_v(p+b(t),x) \neq H_{KH}(p,x+c(t)). \tag{4.25}$$

Note that when in $\eta = e^{q/2}$ the operator q is linear in x or p, the equalities hold in (4.25). Otherwise, the similarity transformation will not induce a simple shift and will mix terms in x and p (for concrete examples, see section 4.2.1).

We will compute the Hamiltonians discussed in section 3 in the velocity and the Kramers-Henneberger gauges, starting from their length-gauge counterparts (Sec. 4.1). Thereby, there exist two ways to proceed: either one applies the gauge transformations $a(t)$ to the Hermitian Hamiltonians $h(t)$, and obtains its non-Hermitian counterpart employing the similarity transformation η, or one applies the transformations $A(t)$ to the pseudo-Hermitian Hamiltonians $H(t)$ directly.

4.2.1 The generalized Swanson Hamiltonian

For the generalized versions of the Swanson Hamiltonian, the similarity transformation η only depends on x, and therefore commutes with the transformation $a_{l\to v}(t)$ from the length to the velocity gauge. This implies that $a_{l\to v}(t) = A_{l\to v}(t)$, so that the Swanson Hamiltonian $H^{S,v}_{n,m}(\alpha,g,t)$ together with its Hermitian counterpart in the velocity gauge are easy to compute

$$H^{S,v}_{n,m}(\alpha,g,t) = \frac{1}{2}\left(p-b(t)\right)^2 + \frac{\alpha}{2}x^n - i\frac{g}{2}(px^{m-1} + x^{m-1}p - 2b(t)x^{m-1}), \tag{4.26}$$

and

$$h^{S,v}_{n,m}(\alpha,g,t) = \frac{1}{2}\left(p-b(t)\right)^2 + \frac{\alpha}{2}x^n + \frac{1}{2}g^2x^{2m-2}, \tag{4.27}$$

respectively.

The computation of the time-dependent Swanson Hamiltonian in the Kramers-Henneberger gauge is slightly more involved, since the gauge transformation $a_{v\to KH}(t)$ no longer commutes with the similarity transformation η. Hence,

$$A_{v\to KH}(t) = \exp[-\frac{g}{m}x^m]e^{id(t)}e^{-ic(t)p}\exp[\frac{g}{m}x^m] \tag{4.28}$$

In this case, the time-dependent Swanson Hamiltonian and its Hermitian counterpart are computed to

$$H^{S,KH}_{n,m}(\alpha,g,t) = \frac{p^2}{2} + \frac{\alpha}{2}(x_c(t))^n + \frac{g^2}{2}(x_c(t))^{2m-2} - i\frac{g}{2}(px^{m-1}+x^{m-1}p) - \frac{g^2}{2}x^{2m-2}, \tag{4.29}$$

and

$$h^{S,KH}_{n,m}(\alpha,g,t) = \frac{p^2}{2} + \frac{\alpha}{2}(x_c(t))^n + \frac{1}{2}g^2(x_c(t))^{2m-2}, \tag{4.30}$$

respectively, with $x_c(t) = x - c(t)$. Note that in this case the equalities in (4.25) do not hold as there are terms in (4.29) occurring for which the displacement $c(t)$ is absent. Such type of terms result from a shift $p \to p - igx^{m-1}$ in the momentum, caused by η. This can be seen explicitly when (4.29) is re-written as

$$H^{S,KH}_{n,m}(\alpha,g,t) = \frac{(p-igx^{m-1})^2}{2} + \frac{\alpha}{2}(x_c(t))^n + \frac{g^2}{2}(x_c(t))^{2m-2}. \tag{4.31}$$

4.2.2 Perturbed anharmonic oscillators

For perturbed anharmonic oscillators, the similarity transformation η depends on p. Hence, it no longer commutes with $a_{l\to v}(t)$, so that

$$A_{l\to v}(t) = e^{-\frac{g}{\alpha}p}e^{ib(t)x}e^{\frac{g}{\alpha}p}. \tag{4.32}$$

On the other hand, such a transformation commutes with $a_{v\to KH}(t)$, from the velocity to the Kramers-Henneberger gauge. Therefore, $A_{v\to KH}(t) = a_{v\to KH}(t)$. For the non-Hermitian Hamiltonians, we then obtain

$$H^{AO,v}_n(\alpha,g,t) = \frac{(p-b(t))^2}{2} + \frac{\alpha}{2}x^n + \frac{i\alpha}{2}\sum_{m=1}^{[\frac{(n+1)}{2}]}\left(\frac{-2g}{\alpha}\right)^{2m-1}\binom{n}{2m-1}\kappa_{2m-1}x^{n+1-2m}$$

$$H^{AO,KH}_n(\alpha,g,t) = \frac{p^2}{2} + \frac{\alpha}{2}x_c(t)^n + \frac{i\alpha}{2}\sum_{m=1}^{[\frac{(n+1)}{2}]}\left(\frac{-2g}{\alpha}\right)^{2m-1}\binom{n}{2m-1}\kappa_{2m-1}(x_c(t))^{n+1-2m}.$$

In this case, the equality sign in (4.25) hold in analogy to their hermitian counterparts (4.24), which is expected, since q is a linear function of p.

Once more we see from this that the non-Hermitian formulation exhibits no advantage over the Hermitian one. Even when in the time independent case the Hamiltonian H is

simpler than its Hermitian counterpart h, this is spoiled by the introduction of the electric field. Thus in such a scenario, we have in h a complicated potential term, but simple dependence on the electric field, whereas in H we have a simple potential but a complicated dependence on the electric field. Alternatively, one could add the field directly to H and thus keep both terms simple, but then the similarity transformation, which is already fixed by the time-independent part, will introduce non-Hermitian terms in h. Apart from this we have seen above that simplicity in the Hamiltonians does not imply simplicity in their eigenfunctions (see section 3.3.3).

4.3 Perturbation theory for non-Hermitian Hamiltonian systems

In most realistic situations, the time evolution of a physical system cannot be computed exactly. For instance, even in a Hermitian framework, it is in general not possible to solve the time-dependent Schrödinger equation for an atomic system with a binding potential $V(x)$ subject to an external laser field $E(t)$. Under these circumstances it is necessary to address the problem perturbatively. In this section, we will show how perturbation theory can be extended to a non-Hermitian framework. As a starting point, let us consider a time-dependent Hermitian Hamiltonian

$$h(t) = h_0(t) + h_p(t) \tag{4.33}$$

where $h_0(t), h_p(t)$ are also Hermitian and satisfy the time-dependent Schrödinger equation. Provided that the time-evolution operators associated to $h(t)$ and $h_0(t)$ both satisfy the relation (4.3), the time evolution operator $u(t,t')$ associated to h can then be expressed by means of Du Hamel's formula [61, 54, 5, 55]

$$u_h(t,t') = u_0(t,t') - i\int_{t'}^{t} u_h(t,s)h_p(s)u_0(s,t')ds. \tag{4.34}$$

By iterating Du Hamel's formula, one obtains a perturbative expansion for the time evolution operator $u_h(t,t')$ in $h_p \ll h_0$. For instance, for a Hamiltonian of an atom in a potential V in the presence of an external laser field

$$h(t) = \frac{p^2}{2} + V(x) + xE(t), \tag{4.35}$$

one chooses $h_p(t) = xE(t)$ and $h_p = V(x)$ in the strong and weak field regime, respectively. In the latter case $h_0(t)$ is the Gordon-Volkov Hamiltonian, i.e., the Hamiltonian of a particle in the presence of the laser field *only* [62, 63].

As we have argued above, relations of the type (4.3) also hold for the time-evolution operator $U(t,t')$ in (4.6). Provided we can sensibly separate $H(t) = H_0(t) + H_p(t)$ such that $U_0(t,t')$ satisfies the relation (4.5) as well, Du Hamel's formula also holds for the non-Hermitian time-evolution operator

$$U_H(t,t') = U_0(t,t') - i\int_{t'}^{t} U_H(t,s)H_p(s)U_0(s,t')ds. \tag{4.36}$$

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

$$\mathcal{P}_{n\leftarrow m} = \left|\langle\Phi_n|\, U(t,0)\, |\Phi_m\rangle_\eta\right|^2 = |\langle\phi_n|\, u(t,0)\, |\phi_m\rangle|^2 \tag{4.37}$$

from an eigenstate $|\phi_m\rangle$ to $|\phi_n\rangle$ of the Hermitian field-free Hamiltonian h or eigenstate $|\Phi_m\rangle$ to $|\Phi_n\rangle$ of the non-Hermitian field-free Hamiltonian H. We will consider first-order perturbation theory with respect to the external laser field amplitude E_0. Iterating (4.34) it follows that to this order the time-evolution operator can be approximated by

$$u^{(1)}(t,0) = u_0(t,0) - i\int_0^t u_0(t,s)xE(s)u_0(s,0)ds, \tag{4.38}$$

where $u_0(t,0) = \exp[-iht]$. The transition amplitude then reads

$$\langle\phi_n|\, u(t,0)\, |\phi_m\rangle = \delta_{nm}e^{-i\varepsilon_n t} - ie^{-i\varepsilon_n t}\,\langle\phi_n|\, x\, |\phi_m\rangle \int_0^t e^{i(\varepsilon_n-\varepsilon_m)s}E(s)ds, \tag{4.39}$$

where the ε_n are the eigenenergies. Form parity considerations it is evident that $\langle\phi_n|\, x\, |\phi_m\rangle \neq 0$ only when m, n are not both even or odd.

Let us now employ these formulae for a concrete examples.

4.4 Harmonic oscillator with a cubic non-Hermitian perturbation

We consider the harmonic oscillator perturbed with a cubic non-Hermitian perturbation in the presence of a laser field

$$H_3^{HO,l}(1,g,t) =: H(t) = \frac{1}{2}p^2 + \frac{1}{2}x^2 + igx^3 + \eta^{-1}x\eta E(t). \tag{4.40}$$

Up to order g^3 this becomes with (3.40)

$$H(t) = \frac{p^2}{2} + \frac{x^2}{2} + xE(t) + ig\left[x^3 + x^2E(t) + 2p^2E(t)\right] + g^2E(t)\left[x^3 - 2pxp\right] + \mathcal{O}(g^3) \tag{4.41}$$

As pointed out earlier, we observe that the additional term in (4.40), which contains the electric field has destroyed the simplicity of the time independent Hamiltonian. There is an additional problem with regard to perturbation theory, because we have lost the clear distinction of the potential term from the electric field term such that the separation into an $H_0(t)$ and $H_p(t)$ becomes more problematic, as now the two parameters g and E_0, which control the perturbative expansion, occur mixed, i.e. one has terms $\propto gE_0$, $\propto g^2E_0$, etc.

The Hermitian setting is much more clear cut and in addition the computations are far simpler as in the free field case the wavefunctions take on a simpler form as discussed in section 3.3.3. Thus when we consider the Hermitian counterpart of (4.41) instead

$$h(t) = h + xE(t) = \frac{1}{2}p^2 + \frac{1}{2}x^2 + g^2\left[\frac{3}{2}x^4 + 3S_{2,2} - \frac{1}{2}\right] + xE(t) \tag{4.42}$$

one is able to overcome this problem. We may now evaluate the transition probability (4.37) for the eigenstates $|\phi_m\rangle$, $|\phi_n\rangle$ of the field-free Hamiltonian $h_3^{HO}(1,g)$ see (3.50), up

to second order in g, such that $u_0(t,0) = \exp[-ih_3^{HO}t]$. Choosing next a concrete form for the laser field $E(t) = E_0 \sin(\omega t)$, that is a monochromatic driving field of frequency ω and field amplitude E_0, we may compute (4.39) for the Hamiltonian (4.42). Our results are presented in figure 1.

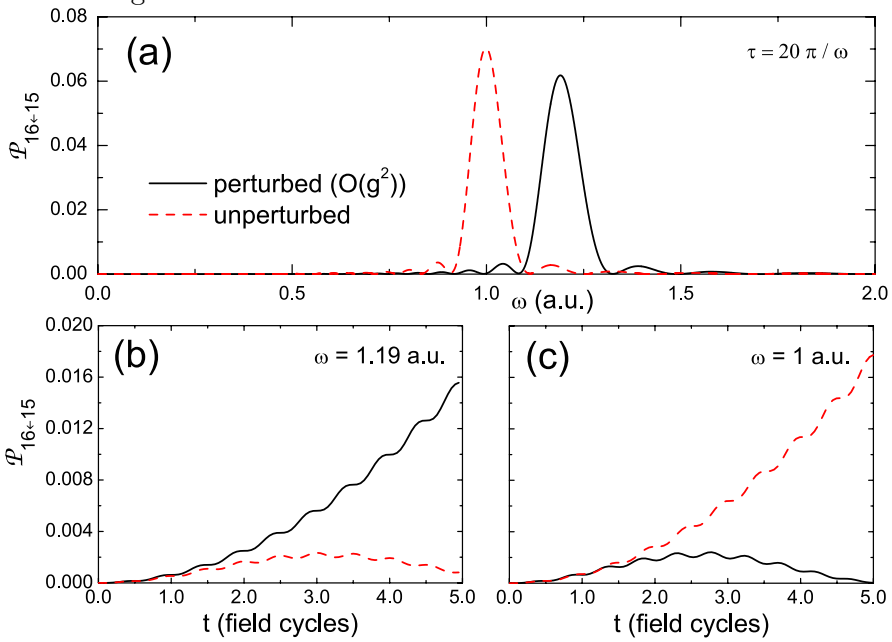

Figure 1: (Color online) Transition probability for a perturbed and unperturbed harmonic oscillator in the presence of a monochromatic laser field, as functions of the field frequency (panel (a)), and of the time (panels (b) and (c)). The perturbed and the unperturbed labels refer to expansions up to second and zero-th order in the parameter g respectively. We consider the transition from the energy level $n = 15$ to $m = 16$ to first-order perturbation theory with respect to the external laser field. The field amplitude is taken to be $E_0 = 0.003$ a.u. and the coupling constant is chosen as $g = 0.04$. The pulse length τ and the frequency ω are indicated in the figure.

Panel (a) displays the transition probabilities $|\phi_{15}\rangle \to |\phi_{16}\rangle$ or $(|\Phi_{15}\rangle \to |\Phi_{16}\rangle)$ up to first order perturbation theory in E_0, when the system is subjected to a pulse of constant duration τ, but with varying field frequency. For comparison, we also consider the unperturbed harmonic oscillator h_0 in the presence of an external laser field, i.e. $h(t)$ in (4.42) for $g = 0$. Our choice of relatively highly excited states is motivated by the fact that according to (3.52) the difference between the perturbed and unperturbed system should be more pronounced for larger values of n.

We expect to find that the system absorbs a single photon of frequency $\omega = \varepsilon_{n+1} - \varepsilon_n$, in order to make a transition from the initial state $|\phi_n\rangle$ to the final state $|\phi_{n+1}\rangle$. Thus for the unpertubed harmonic oscillator we expect a peak at $\omega(h_0) = \varepsilon_{n+1} - \varepsilon_n = 1$ and for the perturbed system we find from (3.52) that the peak should be at

$$\omega(h_3^{HO}, n, g) = \varepsilon_{n+1} - \varepsilon_n = 1 + g^2 \frac{15}{2}(n+1)/2. \tag{4.43}$$

We evaluate from this $\omega(h_3^{HO}, 15, 0.04) = 1.192$, which agrees with our numerical calculation of the expression (4.39), resulting to 1.190.

Next we fix the frequency of the laser field to be resonant with the transition frequency, but vary the duration of the pulse. From standard computations (see e.g. [64]) it follows that the resonance probability should increase with t^2 when the system is tuned to the transition frequency. This behaviour is confirmed by our perturbative calculations. In Panel (b) of figure 1 one clearly observes that that for the perturbed harmonic oscillator, the transition probability increases approximately quadratically in time, whereas the unperturbed system does not exhibit this behaviour as it is off-resonance. In panel (c) the roles of the two systems are exchanged and we are now at the resonance frequency of the unperturbed system whereas the perturbed system is off-resonance.

5. Conclusions

We have constructed various new equivalence pairs, which relate non-Hermitian Hamiltonians to their Hermitian counterparts. Our construction scheme is general and can be employed to compute further pairs not considered this far.

We have demonstrated that when demanding the same similarity transformation to hold for the time-dependent Hamiltonian system and their time-independent counterpart, it is straightforward to develop a framework which describes the time evolution for non-Hermitian Hamiltonian systems. Despite the possibility to compute all relevant quantities in the non-Hermitian framework it turned out that it is usually easier to resort to the equivalent Hermitian formulation of the same systems and perform the evaluations in that context. In the future, it would be very interesting to investigate systems which constitute equivalence pairs in the time-independent case, but have the equivalence relation broken in the time-dependent scenario [59], such as (4.9).

As was already remarked by various authors before, one may question the usefulness of PT-symmetry altogether. First, despite the fact that it is a symmetry, it is does not guarantee that the spectrum of the non-Hermitian Hamiltonian will be real, due to the anti-linear nature of the PT-operator. Second, in the end it will come down to studying pseudo-Hermitian Hamiltonians, which not only constitute a wider class of systems, but in addition do not suffer from the shortcoming that the spectrum might not be positive and real after all. Third, we have used the fact that the time-independent non-Hermitian Hamiltonian is pseudo-Hermitian in formulating the time-evolution operator U. Just having PT-symmetry as the only principle at one's disposal would make this task very difficult. Of course using the relation $\eta^2 = PC$ one may re-express all quantities in terms of CPT-operators, but that would really mean to use the similarity transformations as a construction principle. Fourth, apart from the time-independent Hamiltonian all quantities seem to be simpler in the Hermitian formulation, e.g. see above for the wavefunctions, the time-dependent Hamiltonians in their various gauges and perturbation theory.

Despite its limited constructive power PT-symmetry remains useful in the sense that it is a very simple and transparent property, which can be read off directly from the Hamiltonian and thus constitutes a tool which can be used to identify potentially interesting non-Hermitian Hamiltonians.

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