

The Resonance Phenomena Associated With the Time Asymmetry in Non-Hermitian Quantum Mechanics

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Resonances are defined as the poles of the scattering matrix. The poles are associated with the complex eigenvalues of the Hamiltonian which are embedded in the lower half of the complex plane. The asymptotes of the corresponding eigenfunctions are exponentially diverged. Therefore, the resonance eigenfunctions are not embedded in the Hermitian domain of the Hamiltonian. The time asymmetric problem is discussed for these types of non-Hermitian Hamiltonians and several solutions of this problem are proposed.

KEY WORDS: resonance; time asymmetry; non-Hermitian quantum mechanics.

1. RESONANCES IN NON-HERMITIAN QUANTUM MECHANICS

In the conventional quantum mechanics (QM) the Hamiltonians must be Hermitian. Non-Hermitian Hamiltonians do appear however, in the study of the resonance phenomena (Moiseyev, 1998a; Taylor, 1972) and in other physical contexts (Fogedby *et al.*, 1995; Kadanoff and Swift, 1968; Kim, 1995; Lieb and Wu, 1972; McCoy and Wu, 1968) which are described below.

There are many different reasons for using non Hermitian quantum mechanics. One is to simplify the calculations. There are problems that are quite difficult and sometimes impossible to solve even numerically. For example, when studying the dynamics of molecular systems where the electronic and the nuclear coordinates are strongly coupled to one another and the Born-Oppenheimer approach is not applicable. In such cases the non Hermitian quantum mechanics enables us to take into consideration the coupling between the channels that are open for

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dissociation and ionization in a simple way (Narevich and Moiseyev, 1998, 2000). Another example is studying the dynamics of a system which is coupled to a bath. Often the solution of the full problem is impossible due to the current available computational sources and technology. The calculations become possible by including complex absorbing potential terms (i.e., non Hermitian operators) into the Hamiltonian which introduce the environmental dynamical effects on the studied system (Moiseyev, 1998b; Riss and Meyer, 1993). Another obvious reason to use non Hermitian quantum mechanics is when effects which cannot be described by Hermitian Hamiltonians are to be considered. Such as, diffusion effects, spatial fluctuations in inhomogeneous systems, and effects induced by extended defects in type-II superconductors subject to a tilted external magnetic field (Hatano and Nelson, 1996, 1997, 1998).

For the sake of clarity let us first discuss here the use of non-Hermitian quantum mechanics for calculating the dynamical properties of systems which are prepared in a single resonance state. In hermitian QM a resonance state is *not* an eigenstate of the Hamiltonian but a wavepacket which describes the system in a metastable state. The system in a metastable state has a finite life time. As time passes, the system decays into subsystems. For example, in unimolecular reactions the subsystems are the chemical products. In photoinduced reactions, the subsystems are atomic and/or molecular ions and electrons. In the interaction of atoms with strong laser fields, the subsystems can be the atoms in their ground electronic state and high energy photons (even short wavelengths in the X-ray regime). In scattering experiments of atoms and molecules from solid surfaces, the resonances are desorption states. The wavepacket that describes the resonance phenomena can be expanded in a basis set of eigenfunctions of the Hermitian Hamiltonian. For long living resonances (so called narrow resonances) the dominant contributions to the basis set expansion of the resonance wavepacket are of eigenstates that are embedded in the region of the spectrum where the density states are in particular high.

In non-Hermitian quantum mechanics a resonance state is a pure state. The resonance state is an eigenstate of the Hamiltonian which is solved under the requirement of outgoing boundary conditions. Therefore, the resonance states are associated with complex eigenvalues, $\{E_j = \varepsilon_j - i\Gamma_j/2\}$, with corresponding eigenfunctions that asymptotically are exponentially diverged, $\Psi_j^{\text{res}} \rightarrow \exp(+ik_j r)$ where $k_j \equiv |k_j| \exp(-i\alpha_j) = \sqrt{2mE_j}/\hbar$. Here we assume for the sake of clarity and simplicity but without loss of generality that the potential has a cutoff at the threshold energy $E = 0$. It is clear that the resonance states are *not* embedded in the Hermitian domain of the Hamiltonians and are not in the Hilbert space. It is however possible to carry out a similarity transformation, \hat{S} which will impose on the resonance eigenfunctions exponentially decaying behavior and they will become part of the generalized Hilbert space (in such a case the

definition of the inner product should be generalized as will be discussed briefly later). That is,

$$(\hat{S}\hat{H}\hat{S}^{-1})(\hat{S}\Psi_j^{\text{res}}) = E_j(\hat{S}\Psi_j^{\text{res}}). \tag{1}$$

where,

$$E_j = \varepsilon_j - i\Gamma_j/2 \tag{2}$$

and as $r \rightarrow \infty$ then,

$$\hat{S}\Psi_j^{\text{res}} \rightarrow 0 \tag{3}$$

although,

$$\Psi_j^{\text{res}} \rightarrow \infty. \tag{4}$$

Moiseyev and Hirschfelder have shown that there are infinite types of similarity transformations whereas the complex scaling (i.e., $\hat{S}\Psi(r) = \Psi(r \exp(+i\theta))$) is a specific well known possibility. Other similarity transformations are the exterior scaling and the smooth exterior scaling transformations which are discussed in Hoiseyev (1998a). Let us define the complex scaled Hamiltonian as $\mathcal{H}(\theta) = \hat{S}(\theta)\hat{H}\hat{S}^{-1}(\theta)$. The square integrable eigenfunction of \mathcal{H} are the bound and the resonance states. Bound states implies that $\mathfrak{F}(E) = 0$. The real eigenvalues associated with the bound states and the *complex* eigenvalues associated with the resonance states are θ independent. The corresponding eigenfunctions are varied however with θ . The resonances become square integrable provided that $\theta \geq \alpha$ where $\tan(2\alpha) = \Gamma/(2\varepsilon)$ as defined above (Moiseyev, 1998a). The scattering states are however oscillating non-square integrable functions which are bounded and embedded in the generalized Hilbert space. The eigenvalues associated with the scattering states get complex values which are varied with θ . Such that, $E(\text{scattering}) = |E(\text{scattering}) - E_t| \exp(-2i\theta)$, where E_t stands for the threshold energies. The stationary solutions of the complex scaled Schrödinger equation are given by,

$$\Psi(t) = \exp(-iEt/\hbar)\phi E \tag{5}$$

where,

$$\mathcal{H}(\theta)\phi_E(\theta) = E\phi_E(\theta) \tag{6}$$

where E gets θ independent complex discrete values for the resonances (i.e., complex poles of the Scattering matrix since they are associated with out-going waves and the amplitudes of the incoming waves vanish) and a continuum of complex values which are rotated into the lower half complex energy plane by the angle 2θ .

2. THE TIME ASYMMETRIC PROBLEM AND ITS RELEVANCE TO THE COMPUTATIONS OF MEASURABLE QUANTITIES

It is clear from the discussion given in the previous section that the stationary solutions of the time-dependent Schrödinger equation with complex scaled Hamiltonian are bounded functions (i.e., they do not diverge exponentially in the asymptotic limit) as time increases to $t \rightarrow +\infty$. As a matter of fact if the population of the bound states by the initial wavepacket is zero then $\Psi(t) \rightarrow 0$ as $t \rightarrow \infty$. However, in that case $\Psi(t) \rightarrow \infty$ when $t \rightarrow -\infty$. This is the time asymmetry phenomenon in non-Hermitian QM. In Hermitian quantum mechanics we have the freedom to decide whether as time passes $t \rightarrow \infty$ or $t \rightarrow -\infty$. It is equivalent in some sense to the freedom to choose in what direction the clock hands rotate as time passes. In non Hermitian QM we break the time symmetry requiring that the Hamiltonian has complex eigenvalues which are embedded in the lower half of the complex energy plane. The hands of the clock should move clockwise as time passes when the complex poles and the rotating continuum are in the lower half complex plane and should move anticlockwise as time passes if the complex eigenvalues are in the upper half complex plane.

One may argue that since time is a parameter in the time-dependent Schrödinger equation and therefore any measurable dynamical property is represented by a time-independent operator, one can calculate the probability to measure a given dynamical property and the probability amplitude to get specific products in a time-dependent experiment by using the time-independent scattering theory and avoid the wavepacket time propagation calculations. For non Hermitian QM the complex scaled time-independent scattering theory has been developed. It was also extended to the cases where Hamiltonian is time-dependent. The Hamiltonian becomes time-dependent for example when the system (e.g., atoms or molecules) interacts with electromagnetic fields, that can be induced even by high-intensity short laser pulses. For time-independent complex scaled Hamiltonians, the dynamics is governed by the function $(1 + VG(E))\Phi_0$ where Φ_0 is the complex scaled eigenfunction of the complex scaled Hamiltonian, $\mathcal{H}_0 = \mathcal{H} - V$ and $G = (E - \mathcal{H})^{-1}$. See for example the calculations of Helium diffraction from corrugated copper surfaces and note the remarkable agreement to experimental results (Peskin and Moiseyev, 1993a). For time-dependent Hamiltonian the Green operator within the framework of the (t, t') formalism is given by, $G = (E - [\mathcal{H}(t' - i\hbar \frac{\partial}{\partial t'})])^{-1}$ (Peskin and Moiseyev, 1994). For an example of the use of this formalism see the calculations of the kinetic energy distribution of the ionized electrons of Xenon atoms that were exposed to high-intensity UV radiation (Peskin and Moiseyev, 1993b).

There are cases however where one can not avoid the need to calculate time-dependent expectation values. The amplitude of the probability to measure emitted high frequency radiation due to the nonlinear interaction between atoms or molecules and UV or visible electromagnetic fields is associated with

the Fourier transform of the time-dependent dipole moment, $d(t)$. In non Hermitian QM, $d(t) = (\Psi^L(t)|\hat{d}|\Psi^R(t))$. Let us discuss first the case where $\Psi^R(t)$ and $\Psi^L(t)$ are the right and left solutions of the time-dependent Schrödinger equation when the Hamiltonian is time-independent. The right eigenfunctions of the complex scaled Hamiltonian \mathcal{H} satisfy the equation $\mathcal{H}(\theta)\Phi_j^R = E_j\Phi_j^R$ where $\{E_j\}$ are complex valued. According to definition, the left eigenfunctions of $\mathcal{H}(\theta)$ are associated with the *right* eigenfunctions of $\mathcal{H}^{\dagger*}(\theta)$. It is easy to check that when the Hamiltonian $\mathcal{H}(\theta = 0)$ is real it is true for the complex scaled Hamiltonian that $\mathcal{H}^{\dagger}(\theta) = \mathcal{H}(-\theta) = \mathcal{H}^*(\theta)$ (as an example Hamiltonian one may use $\mathcal{H}(\theta) = \frac{e^{-2i\theta}}{2} \frac{\partial^2}{\partial x^2} + V(x e^{i\theta})$). Therefore, $\Phi_j^L = \Phi_j^R \equiv \Phi_j$. Since the time-dependent wavefunctions satisfy $\mathcal{H}(\theta)\Psi^R(\theta, t) = i\hbar \frac{\partial}{\partial t} \Psi^R(\theta, t)$ and $\mathcal{H}^{\dagger*}(\theta)\Psi^L(\theta, t) = -i\hbar \frac{\partial}{\partial t} \Psi^L(\theta, t)$, it is obvious that the expansion in the basis set Φ_j for the right and left wavefunction is

$$\Psi^R(t) = \sum_j C_j \exp(-i E_j t / \hbar) \Phi_j \tag{7}$$

and

$$\Psi^L(t) = \sum_j C_j \exp(-i E_j t / \hbar) \Phi_j. \tag{8}$$

Since $\Im E_j < 0$ for all eigenstates, except the bound and the threshold states that have real valued eigenvalues, it is clear that $d(t)$ exponentially diverges as $t \rightarrow \infty$ provided the initial wavepacket is *not* in an eigenstate of $\mathcal{H}(\theta)$. In other words the terms that cause the expectation value to diverge exponentially are off-diagonal in the basis set Φ_j (the normalization integral is time-independent).

When the Hamiltonian \hat{H} is time-dependent $\{\Phi_j\}$ and $\{E_j\}$ are replaced respectively by the eigenfunctions and eigenvalues of the complex scaled Floquet like operator, $-i\hbar \frac{\partial}{\partial t} + \mathcal{H}(t', \theta)$.

3. ON THE FERMI'S SOLUTION FOR THE TIME ASYMMETRIC PROBLEM IN NON-HERMITIAN QM

It is clear that time-independent scattering theory for non-Hermitian Hamiltonian can not be derived by solving the time asymmetric problem. An important point in the derivation of time-independent scattering theory for non-Hermitian time-independent Hamiltonians is the use of Lorentzian energy distributions with $-\infty < E < \infty$ that has an exponential time evolution along the positive time propagation direction only. Fermi suggested this approach in order to avoid the nonzero transition probability to excite atom B by absorbing energy emitted by an excited atom A, for time which is smaller than r/c , where r is the distance between the two atoms (Fermi, 1932). This approach however is a consequence of a general theorem (see Bohm *et al.*, 2002; Nicolaides and Beck, 1977a,b and

references therein and also Nicolaidis' contribution to this book). The requirement of $-\infty < E < \infty$ implies that time extends over $0 < t < \infty$ and not over $-\infty < t < \infty$ as in the conventional (Hermitian) quantum mechanics. Therefore Fermi approach seems to break up the time reversal symmetry in non-Hermitian QM. Very recently Bohm and his coworkers have shown that the Fermi's approach does not violate causality when the transformed Fourier is taken for the time-propagated Gamow states (Bohm *et al.*, 2002). The Gamow states, known also as resonance states, are obtained by imposing the Siegert outgoing boundary conditions on the solution of the Schrödinger equation. Therefore, the resonance Gamow states are not in the Hermitian domain of the Hamiltonian and are not in the Hilbert space. They are however embedded in the generalized Hilbert space when they are scaled by a complex factor $\exp(i\theta)$ (Moiseyev, 1998a; Reinhardt, 1982). Upon complex scaling they become square integrable and can be counted by their nodes as regular bound states. The time asymmetry in non-Hermitian QM has been discussed in Bohm *et al.* (2002), Fermi (1932), and Nicolaidis and Beck (1977a,b) for time-independent Hamiltonians. However, using the (t, t') formalism (Peskin and Moiseyev, 1993b) which led us to the derivation of time-independent scattering theory for time-dependent Hamiltonians (Peskin and Moiseyev, 1994), all arguments concerning the time asymmetry problem and its solution hold also for our studied case as well.

For coherency of the analysis we start with a brief introductory comment on the definition of "bra" and "ket" states in non-Hermitian QM when the Hamiltonian is time periodic. The quasi-energy states are time periodic functions. Let us expand them in the Fourier basis set, $f_n \equiv \exp(i\omega n t)$, where $n = 0, \pm 1, \pm 2, \dots$. The Fourier components, ϕ_n, k_{res} , are spatial functions. They are the components of the right eigenvector of the Floquet Hamiltonian matrix, $\mathcal{H}_{n',n} = 1/T \int_0^T dt (f_n'(t))^* [-i\hbar \frac{\partial}{\partial t} + \hat{H}(q \exp(i\theta), t)] f_n(t)$. Where, $\hat{H}(q \exp(i\theta), t) = \hat{H}_{\text{atom/molecule (complex scaled)}} + e\mathcal{E}_0 \exp(+i\theta) \sum_j \hat{z}_j \cos(\omega t)$. Note that in the calculation of the Floquet matrix elements we used the usual scalar product. Without loss of generality we consider the case where the Floquet matrix is equal to its transposed (i.e., \mathcal{H} is a complex symmetric matrix). In such a case the "left" eigenvectors of \mathcal{H} are equal to the "right" one. Therefore, we should not take the complex conjugate of the spatial Fourier components when we calculate expectation values. Consequently, the Floquet eigenstates are orthonormal functions under the definition of: $(1/T) \int_0^T dt \langle \sum_{n'} f_n'(t) (\phi_{n',k_{\text{res}}}(q))^* | \sum_n f_n(t) (\phi_{n,k_{\text{res}}}(q)) \rangle = \delta_{k_{\text{res}},k_{\text{res}}}$. The time period is $T = 2\pi/\omega$ and $\langle \dots \rangle$ stands for the usual definition of the scalar product. Following these formal results we conclude that this definition of the inner product provides a probability to detect the electron *somewhere* in space which is equal to *one* at any given time. This is of course true since the number of particles in the entire space is conserved. However, the high energy photons are generated only due to the interaction of the electrons with the nuclei. On the basis of this physical argument we claim that the number of electrons

should not be conserved inside a finite box where the electrons interact with the nuclei. As time passes, the electrons escape from the finite box. Outside of this finite box we assume that the electron–nuclei interaction is equal to zero. The size of the box can be as large as one wishes. Within the framework of this box quantization formalism the number of the electrons inside the box exponentially decays to zero as time passes. We impose this time-dependent normalization on the quasienergy resonance solutions by introducing the following complex-phase factors: $\exp(-iE_{k'_{\text{res}}}t) = \exp(-i\mathcal{E}_{k'_{\text{res}}}t)\exp(-\frac{1}{2}\Gamma_{k'_{\text{res}}}t)$ for the “ket” Floquet states, and $\exp(+iE_{k_{\text{res}}}^*t) = \exp(+i\mathcal{E}_{k_{\text{res}}}t)\exp(-\frac{1}{2}\Gamma_{k_{\text{res}}}t)$ for the “bra” states. Under this modification the probability to detect the system in a given atomic/molecular quasi-energy resonance (metastable) state, decays exponentially in time. The decay rate is Γ and therefore within the framework of the box-quantization condition mentioned above, $(\Phi_{k_{\text{res}}}(t)|\Phi_{k_{\text{res}}}(t)) = \exp(-\Gamma_{k_{\text{res}}}t)$ when $t = jT$, where $j = 0, 1, 2, \dots$. To obtain this result we used the facts that, $(\dots) = (\exp(-iE_{k_{\text{res}}}t) \sum_{n'} f_{n'}(t)(\phi_{n',k_{\text{res}}}(q))^* | \exp(-iE_{k_{\text{res}}}t) \sum_n f_n(t)\phi_{n,k_{\text{res}}}(q))$; $f_n(t = jT) = \pm 1$; and $\sum_n < (\phi_{n,k_{\text{res}}})^* | \phi_{n,k_{\text{res}}} > = 1$.

This time-dependent normalization for the right and left eigenstates is associated with the Fermi’s approach which enables the derivation of time-independent scattering theory for non-Hermitian (NH) Hamiltonians. However, the question how one can calculate time-dependent expectation values in NH QM without the need to take the Fourier components of the forward time-propagated wavepacket is still unsolved. We can phrase this question in another way. Can one associate the time-dependent “bra” state with the solution of the time-dependent Schrödinger equation with a non Hermitian complex scaled Hamiltonian? The answer to this question is no. Let us explain it:

In Hermitian QM it is well known that the Fourier components of $\Psi(t \rightarrow \pm\infty)$ (with time running forward and backward) are given by,

$$\Psi_E^\pm = \mp i \hat{G}^\pm(E) \Psi(0) \tag{9}$$

where,

$$\hat{G}^\pm(E) = \lim_{\epsilon \rightarrow 0^+} (E - H \pm i\epsilon)^{-1}. \tag{10}$$

It implies that in order to carry out a forward time-propagation in Hermitian QM, a negative imaginary potential term has to be added to the Hamiltonian whereas to get a back-propagation a positive imaginary potential term has to be included in calculations. Since ϵ is a constant parameter it shifts the eigenvalues from the lower half of the complex energy plane to the upper half plane, while the eigenfunctions remain the same. That is,

$$\mathcal{H}(\epsilon)\psi_j = E_j(\epsilon)\psi_j \tag{11}$$

$$\mathcal{H}^*(\epsilon)\psi_j = E_j^*(\epsilon)\psi_j \tag{12}$$

where, $\mathcal{H}(\epsilon) = H - i\epsilon$ and $E_j(\epsilon) = E_j - i\epsilon$. These properties of the non-Hermitian Hamiltonian, \mathcal{H} , allow us to find a relationship between its right and left eigenstates, ψ^R, ψ^L . In the case where both eigenfunctions are real functions (this condition can be always satisfied for the real and Hermitian Hamiltonian \hat{H}), $\psi_j^R = \psi_j^L \equiv \psi_j$. Then the eigenfunction expansion of the time-dependent right and left wavefunctions are

$$\Psi^R(t, \epsilon) = \sum_j C_j \exp(-i E_j(\epsilon)t/\hbar)\psi_j \quad (13)$$

and,

$$\Psi^L(t, \epsilon) = \sum_j C_j \exp(+i E_j^*(\epsilon)t/\hbar)\psi_j \quad (14)$$

where $C_j = \langle \Psi(0) | \psi_j \rangle$ provided that $\Psi(0)$ is a real function as well. The time evolution of an expectation value of an operator \hat{O} is given by,

$$\langle O \rangle (t, \epsilon) = \int_{\text{all-space}} \Psi^L(t, \epsilon) \hat{O} \Psi^R(t, \epsilon) dv / \int_{\text{all-space}} \Psi^L(t, \epsilon) \Psi^R(t, \epsilon) dv \quad (15)$$

Let us return to the non Hermitian complex scaled Hamiltonian $\mathcal{H}(\theta)$. The complex scales operators that are equivalent to $\mathcal{H}(\epsilon)$ and $\mathcal{H}^*(\epsilon)$ are correspondingly $\mathcal{H}(\theta)$ and $\mathcal{H}(-\theta)$. One would be tempted to adopt the expansions in Eqs. (13) and (14) for the complex scaled right and left wavefunctions $\Psi^{R,L}(t)$ with E_j as the eigenvalues of $\mathcal{H}(\theta)$ and E_j^* as the eigenvalues of $\mathcal{H}(-\theta)$. Why this would be wrong? The problem is that contrary to the situation we had before where ψ_j were the eigenfunction of $\mathcal{H}(\epsilon)$ and also of $\mathcal{H}^*(\epsilon)$, the eigenfunctions of $\mathcal{H}(\theta)$, i.e., $\psi_j \equiv \psi_j(\theta)$, are not eigenfunctions of $\mathcal{H}(-\theta)$. Therefore, although it is true that

$$\Psi^R(t, \theta) = \sum_j C_j \exp(-i E_j t/\hbar)\psi_j(\theta) \quad (16)$$

we cannot say on the basis of the above arguments that,

$$\Psi^L(t, \theta) = \sum_j C_j \exp(+i E_j^* t/\hbar)\psi_j(-\theta) \quad (17)$$

since,

$$\psi_j(\theta) \neq \psi_j(-\theta). \quad (18)$$

Note that the coefficients C_j are calculated by projecting the initial complex scaled wavepacket on the eigenfunctions of the complex scaled Hamiltonian. Therefore, $\{C_j\}$ are θ independent. Yet, it is hard to carry out the back rotation transformation in the numerical calculations due to the use of finite number of grid point or finite number of basis functions (Csoto *et al.*, 1990).

Before we continue it is important to remind the reader that the complex eigenvalues E_j can be divided into two sets. One set consists of complex numbers

that are independent of θ (provided θ is sufficiently large). This set contains the resonance complex eigenvalues. The second set consists of complex numbers that depend on θ so that $E_j(\theta) = |E - E_j^{\text{threshold}}| \exp(-2i\theta)$, where $0 \leq E \leq \infty$. The members of the second set are associated with the rotating continuum. As we will see below we can suggest different calculation schemes depending on whether only the resonances or both the rotating continuum and the resonance states are populated by the initial wavepacket.

Alternative approach for studying the dynamics governed by resonance states in NH-QM: As mentioned above we are trying here to look for an approach which is alternative to the known Fermi’s approach. The motivation is the desire to find an approach where the “left” / “bra” time-dependent wavepacket would be obtained by solving the time-dependent non-Hermitian Schrödinger equation when time goes from 0 to $-\infty$. Similar to the evaluation of the “right” / “ket” time-dependent wavepacket the “left” / “bra” time-dependent wavepacket would be obtained by solving the time-dependent non-Hermitian Schrödinger equation when time goes from 0 to $+\infty$.

Our suggestion for calculating time-dependent expectation values when the Hamiltonian is non Hermitian and time-independent is as follows:

1. The “right” time-dependent state (i.e., “ket” state) is the solution of the time-dependent Schrödinger equation with the complex scaled Hamiltonian. The solution is in the generalized Hilbert state (square integrable when only resonances are populated by the initial wavepacket). That is,

$$\Psi^R(t, \theta) = \sum_j^{\text{res}} C_j \exp(-E_j t / \hbar) \psi_j^{\text{res}}(\theta) \tag{19}$$

where,

$$E_j = \epsilon_j - i\Gamma_j/2. \tag{20}$$

and,

$$\theta \geq 0.5 \arctan \left((\epsilon_j - E_j^{\text{threshold}}) / (\Gamma_j/2) \right). \tag{21}$$

2. The “left” time-dependent state (i.e., the “bra” state) is obtained in two steps:
 - I. The wavepacket at time zero is propagated *backward* in time, using the complex conjugate of the complex scaled Hamiltonian given in our case by $\mathcal{H}(-\theta)$. The time-dependent solution can be expressed as (compare with Eq. (17)),

$$\Phi(t, -\theta) = \sum_j^{\text{res}} C_j \exp(+i E_j^* t / \hbar) \psi_j^{\text{res}}(-\theta) \tag{22}$$

where,

$$E_j^* = \epsilon_j + i\Gamma_j/2. \quad (23)$$

and as before,

$$\theta \geq 0.5\theta_c \quad (24)$$

where,

$$\theta_c \equiv \arctan((\epsilon_j - E_j^{\text{threshold}})/(\Gamma_j/2)). \quad (25)$$

In spite of the fact that we rotate the coordinates into the complex energy plane by the angle $-\theta$ rather than $+\theta$ we require the solution to be square integrable. Note that in the summary section of this manuscript we call $\Phi(t, -\theta)$ wavefunction a $\Psi^{\text{“L”}}$ state. The quotation marks here imply that “L” is *not* a left/bra state.

- II The “bra”/“left” state is obtained by carrying out analytical continuation of $\Phi(t, -\theta)$ in parameter θ using for example Padé approach. Analytically continuing the complex function $\Phi(t, -\theta)$ calculated for $\theta \geq \theta_c$, one gets the complex scaled function $\Phi(t, \theta)$ such that,

$$\Psi^{\text{L}}(t, \theta) \equiv \Phi(t, \theta) = \sum_j^{\text{res}} C_j \exp(+iE_j^*t/\hbar)\psi_j^{\text{res}}(+\theta). \quad (26)$$

Following the procedure given above the normalization conditions are redefined in such a way that every one of the resonance eigenstates is no longer normalized to unity. Instead they are normalized to a time-dependent factor which decays exponentially in time, so that,

$$\int_{\text{all-space}} \Psi^{\text{L}}(t, \theta)\Psi^{\text{R}}(t, \theta) = \sum_j^{\text{res}} (C_j)^2 \exp(-\Gamma_j t/\hbar). \quad (27)$$

It is easy to extend this approach to time-dependent Hamiltonians using the (t, t') formalism (Peskin and Moiseyev, 1993b). Then the complex scaled Hamiltonian $\mathcal{H}(\theta)$ is replaced by the Floquet type operator $\mathcal{H}_f(\theta) \equiv -i\hbar \frac{\partial}{\partial t'} + \mathcal{H}(t', \theta)$. The eigenfunctions of $\mathcal{H}_f(\theta)$ are the quasi-energy states and can be expanded in variable t' Fourier basis functions. The photo induced resonances are θ independent exactly as in the cases where the Hamiltonian is time-independent. A right resonance eigenstate (i.e., “ket”) is an eigenfunction of $\mathcal{H}_f(\theta)$ multiplied by $\exp(-iE_{\text{res}}t/\hbar)$, where E_{res} is the corresponding eigenvalue. A left/“bra” state is an analytically continued eigenfunction of the complex conjugate of $\mathcal{H}_f(-\theta)$ multiplied by $\exp(+iE_{\text{res}}^*t/\hbar)$. Using this formalism we are able to derive an expression for the high-order harmonic generation spectra.

Alternative approach for studying the dynamics governed by the most general case where both resonance and scattering states are populated by the initial

wavepacket: The analytical continuation of the wavepacket obtained by the backward in time propagation calculations, $-\theta \rightarrow +\theta$, succeeds to generate the left/bra state given in Eq. (26) due to the fact that the resonance complex eigenvalues are θ independent. However, the complex eigenvalues associated with the rotating continuum depend on θ and under the analytical continuation will transform from $\exp(+i E^*(\text{complex})t/\hbar) = \exp(+i|E| \cos(2\theta)t/\hbar) \exp(-|E| \sin(2\theta)t/\hbar)$ to $\exp(+i E(\text{complex})t/\hbar) = \exp(+i|E| \cos(2\theta)t/\hbar) \exp(+|E| \sin(2\theta)t/\hbar)$ which diverges exponentially as $t \rightarrow \infty$. To overcome this difficulty we propose here:

1. To carry out the analytical continuation in θ of the relevant expectation values, rather than analytically continuing $\Phi(t, -\theta)$ as defined in Eq. (22),

$$\langle O \rangle(t, \theta) \equiv \frac{\int_{\text{all-space}} \Phi(t, -\theta) \hat{O}(\theta) \Psi^R(t, \theta) dr}{\int_{\text{all-space}} \Phi(t, -\theta) \Psi^R(t, \theta) dr}, \tag{28}$$

where $\hat{O}(\theta)$ is a complex scaled operator.

2. To carry out the analytical continuation of $\langle O \rangle(t, \theta)$ from $\theta > \theta_c$ to $\theta = 0$.

The idea is clear. By rotating back the complex coordinate to the real axis the scattering/continuum states acquire real eigenvalues as usual and are in the Hilbert space, whereas the resonance states have complex eigenvalues and eigenfunctions that diverge exponentially and do not belong to the Hermitian domain of the Hamiltonian and are not in the Hilbert space. The “trick” is that we rotate backward the coordinate by carrying out analytical continuation of $\langle \hat{O} \rangle(t, \theta)$ to $\langle \hat{O} \rangle(t, \theta = 0)$. Therefore, in spite of the fact that the resonance eigenfunctions diverge exponentially at $\theta = 0$ the integrals converge because when we calculate them at $\theta \neq 0$ the integrands are zero at $\pm\infty$.

4. SUMMARY

Resonances are defined as the poles of the scattering matrix. The poles are associated with the complex eigenvalues of the Hamiltonian embedded in the lower half of the complex plane. The asymptotes of the corresponding eigenfunctions are exponentially diverged. Therefore, the resonance eigenfunctions are not embedded in the hermitian domain of the Hamiltonian. Upon complex scaling, however, the resonance eigenfunctions become square integrable. Here we argue that when the complex scaled Hamiltonian is denoted by $\mathcal{H}(\theta)$ where $\exp(i\theta)$ is the complex scaled parameter, then the time-dependent expectation value of the dynamical quantity O is given by the absolute value of $\lim_{\theta \rightarrow 0} \langle \hat{O} \rangle_\theta$. The limit $\theta \rightarrow 0$ is taken using the Padé extrapolation procedure. The complex quantity $\langle \hat{O} \rangle_\theta$ is calculated for sufficiently large value of θ to make the resonance states which are populated by the initial wavepacket to be square integrable. The complex analog of the expectation value of \hat{O} is defined as

$(\Psi^{\text{L}}(\theta, t)|\hat{O}|\Psi^{\text{R}}(\theta, t))\Psi^{\text{R}}(\theta, t)$. and $\Psi^{\text{L}}(\theta, t)$ are correspondingly the solutions of the right and left time-dependent Schrödinger equations which are defined as: $\mathcal{H}(\theta)\Psi^{\text{R}}(\theta, t) = i\hbar\frac{\partial}{\partial t}\Psi^{\text{R}}(\theta, t)$ and $\mathcal{H}(-\theta)\Psi^{\text{L}}(\theta, t) = -i\hbar\frac{\partial}{\partial t}\Psi^{\text{L}}(\theta, t)$. The initial conditions are defined such that at $t = 0$, Ψ^{R} is the complex scaled initial wavepacket, $\hat{S}(\theta)\Phi_0$ whereas $\Psi^{\text{L}}(t = 0) = \hat{S}(-\theta)\Phi_0$. By using the (t, t') method as formulated by Peskin and Moiseyev this formulation of the non-Hermitian QM is immediately applicable also for cases where the Hamiltonian is time-dependent, regardless if the dependent potential is periodic in time or not. Here we assumed for the sake of simplicity but without loss of generality that the nonscaled Hamiltonian $\hat{\mathcal{H}} = \mathcal{H}(\theta = 0)$ is real.

To avoid the need to extrapolate $(\hat{O})_\theta \equiv \langle \hat{O} \rangle(\theta)$ to $\theta = 0$ one can use as a new orthonormal basis set the eigenfunctions of the unscaled Hamiltonian which are in the Hilbert space and the resonance eigenfunctions which are obtained by imposing outgoing wave boundary conditions on the solutions of the Schrödinger equation. The definition of the inner product should be modified as described above.

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