Weak measurements in non-Hermitian systems

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Abstract

‘Weak measurements’—involving a weak unitary interaction between a quantum system and a meter followed by a projective measurement—are investigated when the system has a non-Hermitian Hamiltonian. We show in particular how the standard definition of the ‘weak value’ of an observable must be modified. These studies are undertaken in the context of bound-state scattering theory, a non-Hermitian formalism for which the involved Hilbert spaces are unambiguously defined and the metric operators can be explicitly computed. Numerical examples are given for a model system.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The standard formulation of quantum mechanics requires physical observables to be mathematically given in terms of Hermitian operators. In the last decade, theories with a non-Hermitian Hamiltonian have been extensively investigated [1]. The initial momentum was given by work concerning PT-symmetric Schrödinger operators [2]. It was hoped that the PT-symmetric Hamiltonians, which are complex but nevertheless possess a real spectrum, would provide an extension of standard quantum mechanics. It was later argued however that these non-Hermitian operators could be mapped to Hermitian ones by a similarity transform [3]. Nevertheless the non-Hermitian framework remains useful. Indeed, from a fundamental perspective, it opens up the possibility of doing quantum mechanics with non-standard inner products. This has practical consequences because many physical systems are naturally formulated in non-Hermitian terms [4].

Scattering systems involving bound states in real potentials are such a case. While scattering problems in complex potentials have been prominent in the studies of non-Hermitian Hamiltonians, bound-state scattering in short-range real potentials has been scarcely
investigated [5–7]. In this case, non-Hermiticity arises from the boundary conditions imposed on the scattering functions, ultimately linked to the fact that the scattering solutions are not the full eigenstates of the exact Hamiltonian. From the physical point of view, this exact Hamiltonian exists, but its eigenstates are unknown in practice, while the bound scattering solutions are the eigenstates of an effective Hamiltonian that is not Hermitian relative to the standard inner product. Hence, in principle, one should employ a bi-orthogonal basis or equivalently obtain the metric operator in order to define the inner product relative to which the effective Hamiltonian becomes self-adjoint (in practice, this issue is ignored in the most widely employed application of bound-state scattering, namely the computation of the spectrum of the excited electronic states of atoms and molecules, an ignorance that can be justified by the fact that in most cases the non-Hermiticity index is very small, see section 4.1).

In this paper, we will focus on the interaction between a bound-state scattering system and a measurement device in a scheme popularly known as ‘weak measurements’ (WM). WM, introduced more than two decades ago [8], have been receiving increased attention in the last five years, in particular as a theoretical and also experimental tool aimed at investigating fundamental problems in quantum mechanics (see [9] and references therein). WM actually involve two steps: the first step is a weak interaction between the system and a ‘weak meter’, the overall evolution being unitary. The second step is a standard projective measurement in which the system (at that point entangled with the weak meter) interacts with a different measurement device. The state of the system is projected to a final post-measurement state, while the weak meter has picked up a phase depending on a quantity known as the ‘weak value’ of the weakly measured observable. In the conjugate variable of the pointer, the phaseshift appears as a shift in the probability distribution. This shift can be experimentally measured by obtaining the probability distribution of the weak pointer.

The main issue when considering a WM of a non-Hermitian system lies in the treatment of the coupling between the system and the weak meter. Indeed in a standard projective measurement, the observed quantity is an eigenvalue, which is a real quantity not depending on the definition of the inner product. In a WM, the observed quantity is a shift in the pointer proportional to the weak value, which, as will be seen below, is a renormalized transition element. It is therefore crucial, in order to determine the weak value, to properly define the inner product and the physical Hilbert space.

We first briefly introduce WM and give the usual formula for computing weak values (section 2). We then derive the weak value for non-Hermitian systems. In order to provide an unambiguous physical basis, this derivation will be done in the context of bound-state scattering theory. We thus explain why systems described with this formalism are non-Hermitian in the ‘physical’ Hilbert space, leading to the definition of a new inner product and its associated Hilbert space, in which the weak values must be defined (section 3). We then give in section 4 examples of weak value computations for a model bound scattering system. We see that non-Hermitian issues must be incorporated explicitly in order to account for the correct shift in the WM apparatus. Our concluding remarks are given in section 5.

2. Weak measurements

A standard quantum measurement, often represented by the projection of a pre-measurement state of the system to an eigenstate of the measured system observable, actually involves a two-step procedure. First, a unitary interaction between the measured system and the measurement apparatus results in a system–apparatus state entangled in the pointer basis. Then, in a second step, the entangled state is projected to a final post-measurement state correlating a unique pointer state with an eigenstate of the measured observable.
A WM of an observable $A$ proceeds differently. First, a weak unitary interaction takes place between the system and the ‘weak’ meter. The weakness of the interaction results in an entanglement [10] in which the different pointer states are nearly identical. Then, a standard quantum measurement of a different observable takes place, resulting in the usual projection to an eigenstate of this second observable. Since the system and the weak apparatus were still entangled, the projection to a final state of the system also determines the quantum state of the weak meter.

Rather than solving for the weak interaction in terms of the entangled states in the pointer basis, the standard approach [8] to WM starts from a first-order expansion of the interaction Hamiltonian. Let $|\psi(t_i)\rangle$ and $|\Phi(t_i)\rangle$ be the initial states of the system and weak meter, respectively, just before they interact, and let us assume an interaction Hamiltonian of the form $I(t) = f(t)AX$, where the system observable $A$ is coupled to the weak pointer’s position variable along the $x$-axis (i.e. $X[X] = X[X]$ for the pointer). $f(t)$ is a smooth function of $t$ vanishing outside the interval $t_- < t < t_+$ during which the interaction takes place and obeying $\int_{t_-}^{t_+} f(t) \, dt = g$, where $g$ is the mean effective coupling strength. Neglecting the self-evolution of the system and meter during the time interval $t_- - t_-$, the unitary evolution generated by $I(t)$ brings the initial state $|\Psi(t_i)\rangle \equiv |\psi(t_i)\rangle |\Phi(t_i)\rangle$ to

$$
|\Psi(t_+)\rangle = e^{-igAX} |\psi(t_i)\rangle |\Phi(t_i)\rangle.
$$

(1)

A projective measurement of another observable $B$ of the system is made immediately after. The system state is projected to one of the eigenstates of $B$; among the possible outcomes, we select only the cases in which the final state is $|\beta_f\rangle$. The standard approach consists in expanding the exponential to first order in $g$ and then computing the projection

$$
\langle X | (|\beta_f\rangle |\psi(t_i)\rangle) \simeq (|\beta_f\rangle |\psi(t_i)\rangle) \langle X | \exp \left( -ig \frac{\langle \beta_f | A | \psi(t_i) \rangle}{\langle \beta_f | \psi(t_i) \rangle} AX \right) |\Phi(t_i)\rangle.
$$

(2)

The term

$$
\langle A \rangle_W \equiv \frac{\langle \beta_f | A | \psi(t_i) \rangle}{\langle \beta_f | \psi(t_i) \rangle}
$$

(3)

is known as the weak value of $A$. Equation (2) indicates that the weak meter has picked up a phase (in configuration space), or alternatively a shift (in momentum space) proportional to the weak value of $A$, given the initial (known as ‘preselected’) state, and the final (known as ‘postselected’) state obtained after having made a standard measurement of another observable $B$. Note that the weak value can be a complex number, implying that different shifts can be observed in the conjugate variables of the meter [11].

The derivation of equation (2) involves several approximations (see, e.g., [10]) that will not be discussed here. A necessary (but not sufficient) condition is that $g\langle A \rangle_W$ is small, generally implying that the coupling $g$ must be vanishingly small (because $\langle A \rangle_W$ is generally large). The important point, from a physical perspective, is that measuring the weak meter wavefunction allows one to obtain information, encoded in $\langle A \rangle_W$, on the system observable $A$ without making a full quantum measurement of that observable. Instead another, possibly incompatible property $B$ is measured.

The applications and interpretations of WM are out of the scope of this work. Our focus here lies in the WM of a system described in a non-Hermitian framework. Indeed, accounting for WM involves treating—though only to first order—the interaction between the non-Hermitian system and a measurement device. Contrary to a standard measurement, in which case the outcome would be an eigenvalue, the measurement device is shifted by the weak value. However, definition (3) of the weak value is valid in standard (Hermitian) quantum mechanics. For a system described in a quasi-Hermitian framework, $\langle A \rangle_W$ must be
computed in the correct Hilbert space, endowed with a non-standard inner product, as will be seen below.

3. Non-Hermitian formalism

3.1. General remarks

The weak value as given by equation (3) needs to be modified for systems described in a non-Hermitian setting. The rationale, well-known to practitioners of PT-symmetric/quasi-Hermitian quantum mechanics, is that the inner product needs to be replaced. Given the controversies surrounding the physical interpretation of non-Hermitian systems [12], our approach will consist in working with a system—or rather a family of systems, those involving bound-state scattering—that has an important advantage: the non-Hermitian aspects appear because one is led to work with wavefunctions defined on a modified configuration space. This means that while the scattering Hamiltonian is non-Hermitian, there is in principle an underlying exact Hamiltonian (though intractable in practice). As a result there is no ambiguity when dealing with the conceptual aspects surrounding non-Hermiticity.

We will therefore first give a brief presentation on bound-state scattering, exposed previously in [5], and discuss its non-Hermitian aspects in order to derive the formula for the weak value in non-Hermitian systems, given by equation (24).

3.2. Bound-state scattering

For definiteness, let us consider two particles, a light particle and a massive compound target, attracted by a long-range radial field. The scattering between the particles is described by a short-range potential. Letting $H^c$ denote the exact Hamiltonian in the center of mass, we assume $H^c$ can be split as

$$H^c = H_0 + V,$$

where $H_0$ is the Hamiltonian of the light particle in the long-range field and $V$ contains all the short-range interactions between the light particle and the target. We further assume that

$$\langle r' | V | r \rangle = \theta (r_0 - r') V \theta (r_0 - r),$$

i.e. $V$ vanishes outside some small radius $r_0$ ($\theta$ is the step function). The total energy $E$ can be partitioned as

$$E = \epsilon_i + \epsilon_f,$$

where $\epsilon_i$ is the internal energy of the target (depending on the target quantum state) and $\epsilon_f$ is the energy of the light particle. The eigenstates of $H_0$ are given by

$$|\phi_i(E)\rangle = |f_i(\epsilon_i)\rangle|i(\epsilon_i)\rangle;$$

$$f_i(\epsilon_i, r) \equiv \langle r | f_i(\epsilon_i) \rangle$$

is the eigenfunction of the radial part of $H_0$, whereas the ‘target’ state $|i(\epsilon_i)\rangle$ includes all the other degrees of freedom, including the non-radial ones of the colliding particle (a handy notation given that the angular momenta of the particles are usually coupled). The target states are orthogonal, $\langle i | j \rangle = \delta_{ij}$. For bound states, $f_i(\epsilon_i, r)$ vanishes at 0 and $+\infty$ (whenever $E$ is an eigenvalue of $H_0$).

The label $i$ defines the scattering channel. In each channel, the standing-wave solutions are given by the Lippmann–Schwinger equations of scattering theory as

$$|\psi_f^i(E)\rangle = |\phi_i(E)\rangle + \alpha G_0(E)K(E)|\phi_i(E)\rangle,$$
where $G_0(E)$ is the principal-value Green’s function and $K$ is the reaction (scattering) operator for standing waves linked to the familiar $S$ matrix by a Cayley transform [13] (the scattering matrix is assumed to be known). The difference here from standard scattering theory is that the bound channels are included explicitly\(^1\). Both $\langle r \mid \phi_i(E) \rangle$ and $\langle r \mid \phi'_i(E) \rangle$ diverge as $r \to \infty$ for an arbitrary value of $E$. A bound state appears when the superposition

$$|\psi^r(E)\rangle = \sum_i Z_i(E)|\psi'_i(E)\rangle$$

converges as $r \to \infty$. This happens for discrete values of the energy obtained, along with the expansion coefficients $Z_i(E)$, by imposing the boundary conditions.

While $H^r$ is undoubtedly Hermitian relative to the standard inner product, its eigenfunctions cannot be computed from equations (8) and (9) because the formal expansion of $G_0$ over the eigenstates of $H_0$ is intractable. Instead the scattering formulation consists in obtaining a closed-form expression of $G_0$ valid only outside the reaction zone, i.e. for $r > r_0$. Indeed from the scattering viewpoint, whatever happens within the reaction zone is encoded in the phaseshifts. The wavefunction (9) outside the reaction zone takes the form

$$\langle r \mid \psi(E)\rangle = \sum_i Z_i(E) \left[ f_i(\epsilon_i, r)|i\rangle + \sum_j g_j(\epsilon_j, r)|j\rangle K_{ji} \right], \quad r > r_0,$$

where $K_{ji}$ are the on-shell elements of the scattering matrix, which are assumed to be known. $g(r)$ is, like $f(r)$ introduced in equation (7), a solution of the radial part of $H_0$ but it is irregular at the origin.

The scattering state $|\psi(E)\rangle$ of (10) is the part for $r > r_0$ of the exact solution $|\psi^r(E)\rangle$ and not an approximation to it. But within the scattering formulation, the ‘inner’ part of $|\psi^r(E)\rangle$ for $r < r_0$ does not exist: all meaningful quantities are defined radially on $[r_0, \infty]$. As a consequence,

$$\langle \psi(E_1) \mid \psi(E_2) \rangle = \delta_{E_1 E_2} + \mu_{E_1 E_2} (1 - \delta_{E_1 E_2}),$$

i.e. the scattering states are normalized to 1, but are not orthogonal; this is due to the fact that the boundary conditions at $r = r_0$ are not identical for all $|\psi(E)\rangle$ [5]. Hence, the scattering states cannot be eigenstates of the Hermitian operator

$$H = \sum_E E |\psi(E)\rangle \langle \psi(E)|,$$

since $H|\psi(E)\rangle \neq E|\psi(E)\rangle$. A non-Hermitian Hamiltonian needs to be introduced instead.

3.3. Non-Hermitian aspects: metric, Hilbert spaces and operators

Let $\mathcal{H}_\text{ph}$ be the Hilbert space of standard quantum mechanics. Physical states are represented by vectors in $\mathcal{H}_\text{ph}$. From a practical viewpoint, we may consider that the phaseshifts (or the $K$ matrix elements) are known and the problem concerns the expansion of physical states in terms of the scattering solutions $|\psi(E)\rangle$.

To this end, let us introduce a non-Hermitian operator $\tilde{H}$ and state vectors $|\tilde{\psi}(E)\rangle$, such that

$$\tilde{H}|\tilde{\psi}(E)\rangle = E|\tilde{\psi}(E)\rangle,$$

$$\tilde{H}^\dagger|\tilde{\psi}(E)\rangle = E|\tilde{\psi}(E)\rangle,$$

\(^1\) This means that $G_0(E)$ is modified relative to the usual resolvent by including a term canceling the poles at the eigenvalues of $H^r$ [14].
\[ \langle \tilde{\psi}(E)|\psi(E') \rangle = \delta_{EE'}, \]  
(15)
where \(|\tilde{\psi}(E)\rangle, |\psi(E)\rangle\) forms a bi-orthogonal basis. It follows that we can write the following expansions:
\[ \tilde{H} = \sum_{E} E|\psi(E)\rangle\langle \tilde{\psi}(E)|, \quad \tilde{H}^+ = \sum_{E} E|\tilde{\psi}(E)\rangle\langle \psi(E)|. \]  
(16)

\(\tilde{H}\) and \(\tilde{H}^+\) are further linked by
\[ \tilde{H} = \mathcal{G}\tilde{H}^+\mathcal{G}^{-1}, \]  
(17)
where \(\mathcal{G}\) is a Hermitian operator given by
\[ \mathcal{G} = \sum_{E} |\psi(E)\rangle\langle \psi(E)|, \quad \mathcal{G}^{-1} = \sum_{E} |\tilde{\psi}(E)\rangle\langle \tilde{\psi}(E)|. \]  
(18)

Equation (17) is the defining relation of quasi-Hermiticity [15], with \(\mathcal{G}\) being invertible and positive definite [5].

This allows one to define a Hilbert space \(\mathcal{H}\) endowed with a new inner product depending on the metric \(\mathcal{G}\):
\[ (\psi(E_1), \psi(E_2)) = \langle \psi(E_1)|\mathcal{G}^{-1}|\psi(E_2) \rangle = \langle \tilde{\psi}(E_1)|\tilde{\psi}(E_2) \rangle = \delta_{E_1E_2}, \]  
(19)

Equation (17) indicates that \(\tilde{H}\) is Hermitian relative to this new inner product. Completeness of the bi-orthogonal basis allows one to expand an arbitrary state of \(\mathcal{H}_{ph}\) in terms of the \(|\psi(E)\rangle\), i.e. the eigenstates of \(\tilde{H}\) span the entire Hilbert space of admissible physical states even if they do not form an orthogonal basis in \(\mathcal{H}_{ph}\).

Calculations involving the scattering states have to be performed in \(\mathcal{H}\) rather than in \(\mathcal{H}_{ph}\). Indeed although a physical state \(|\alpha_k\rangle_{ph}\) is known in \(\mathcal{H}_{ph}\), its expansion over the scattering eigenstates \(|\alpha_k\rangle = \sum_{E} a_k(E)|\psi(E)\rangle\) is defined in \(\mathcal{H}\) with the expansion coefficients given through
\[ a_k(E) = \langle \tilde{\psi}(E)|\alpha_k \rangle \equiv (\psi(E), \alpha_k)_{\mathcal{G}} = \langle \psi(E)|\tilde{\alpha_k} \rangle, \]  
(20)
where we have put \(|\tilde{\alpha_k}\rangle = \mathcal{G}^{-1}|\alpha_k\rangle\). Note that in the underlying exact problem, there is a physical state corresponding to \(|\alpha_k\rangle\) and given by the same expansion coefficients but over the eigenstates of the exact Hamiltonian, \(|\alpha'_k\rangle = \sum_{E} a_k(E)|\psi'(E)\rangle\), with \(a_k(E) = \langle \psi'(E)|\alpha'_k \rangle\).

We can therefore understand non-Hermiticity as a consequence of working with exact wavefunctions but defined only over part of configuration space relative to the underlying exact problem.

As was the case with \(H\) (see equation (12)) that needed to be replaced with \(\tilde{H}\), an operator \(A\) Hermitian in \(\mathcal{H}_{ph}\), is represented in \(\mathcal{H}\) by an operator \(\mathcal{A}\) whose expansion over the bi-orthogonal basis reads
\[ \mathcal{A} = \sum_{EE'} |\psi(E)\rangle\langle \psi(E')| \tilde{A}_{EE'} |\tilde{\psi}(E')\rangle, \]  
(21)

The relation between \(A\) and \(\tilde{A}\) is given by [15, 5] \(A = \mathcal{G}^{-1/2}\tilde{A}\mathcal{G}^{1/2}\). The time evolution operator is a prominent example: \(U(t) = \sum_{E} e^{-iE't}|\psi(E)\rangle\langle \psi(E)\rangle\) is not unitary in \(\mathcal{H}_{ph}\). The correct unitary operator in \(\mathcal{H}_{ph}\) is obtained from \(U = \mathcal{G}^{-1/2}\tilde{U}\mathcal{G}^{1/2}\), where \(\tilde{U}(t)\) defined by
\[ \tilde{U}(t) = \sum_{E} e^{-iE't}|\tilde{\psi}(E)\rangle\langle \tilde{\psi}(E)| \]  
(22)
is (pseudo) unitary in \(\mathcal{H}\).

\(^2\) We will not address here the delicate technical aspects related to completeness in the case of infinite-dimensional Hilbert spaces.
3.4. Weak values

We are now in a position to formulate the weak value expression for a non-Hermitian system. First note that, as described in section 2, we do not need to solve explicitly the full problem involving the coupling of a non-Hermitian system to a Hermitian one (as e.g. in [16]). Indeed the non-Hermitian system is practically not affected by the weak interaction, while the Hermitian one (the meter) simply picks up a phase. This phase—the weak value—is therefore the only quantity that we need to determine.

Let $|\alpha_i\rangle = \sum E a_i(E) |\psi(E)\rangle$ be the initial (‘preselected’) state prior to the WM of a system observable $A$ and $|\beta_f\rangle = \sum E b_f(E) |\psi(E)\rangle$ be the ‘postselected’ state obtained after the subsequent projective measurement. According to the discussion above, $|\alpha_i\rangle$ and $|\beta_f\rangle$ represent the physical states in $\mathcal{H}$ and the coefficients $a_i$ and $b_f$ are given by formulas analogous to equation (20). The observable $A$ is represented in $\mathcal{H}$ by the non-Hermitian operator $\tilde{A}$ whose expansion over the bi-orthogonal basis was given by equation (21).

Formula (3) expressing the weak value of the observable $A$ becomes

$$\langle \tilde{A} \rangle_W = \frac{\langle \beta_f | \tilde{A} | \alpha_i \rangle_G}{\langle \beta_f | \alpha_i \rangle_G} \quad (23)$$

or in terms of the standard inner product notation

$$\langle \tilde{A} \rangle_W = \frac{\langle \tilde{A} | \tilde{A} | \alpha_i \rangle}{\langle \beta_f | \beta_f \rangle} = \frac{\langle \beta_f | G^{-1/2} \tilde{A} | \alpha_i \rangle}{\langle \beta_f | G^{-1/2} | \alpha_i \rangle} = \frac{\langle \beta_f | G^{-1/2} A G^{-1/2} | \alpha_i \rangle}{\langle \beta_f | G^{-1} | \alpha_i \rangle}. \quad (24)$$

Hence, when a system that is non-Hermitian (relative to the standard inner product) interacts with a WM apparatus measuring the observable $A$, the meter is shifted by a quantity given by equation (24), not by equation (3); equations (24) and (3) obviously coincide when the metric is flat ($G$ is the identity operator). Note that the shift in the WM apparatus can in principle be experimentally observed.

4. Computation of weak values in a model non-Hermitian system

4.1. Model

We will give examples involving the computation of equation (24) in a situation well known in atomic physics involving atoms or molecules with a single excited electron (known as ‘Rydberg’ atoms or molecules). In this case, the long-range field is the familiar Coulomb potential and the reaction zone is about the size of the atomic core. The excited electron periodically scatters off the core, the core–electron interaction being embodied in the short-range potential. We set up a model with five scattering channels: the target has a ground state with $\epsilon_1 = 0$ and four excited states with energies $\epsilon_i, i = 2, \ldots, 5$. We choose the elements of the $5 \times 5$ scattering matrix $K(E)$ to have a very strong energy dependence in order to have stronger non-diagonal elements of the metric $G$. A non-Hermiticity index $\kappa$ quantifying how much $G$ departs from the flat metric can be defined [5] by averaging over the $N$ largest non-diagonal elements of $G$, where $N$ is the dimension of the metric. In this model, we have $\kappa = 0.061$, a relatively small value that is however five or six orders of magnitude larger than the value of $\kappa$ for typical ‘Rydberg’ atoms or molecules. This is why in most cases non-Hermitian issues can (and have been) ignored when computing the spectrum of the

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3 For Rydberg atoms or molecules, $K(E)$, adjusted from experimental data or determined through highly demanding many-body computations in the reaction zone, generally has a mild energy dependence.

4 In certain cases, e.g., when the problem involves the computation of reduced density matrices, an ad hoc renormalization needs to be done given that the norm is not conserved even in typical cases; taking into account non-Hermiticity in order to conserve the norm is a better option [17].
Rydberg states—a negligible κ meaning $G$ is nearly identical to the identity matrix. Therefore, the present model can hardly claim to represent a typical Rydberg problem, though scattering matrices corresponding to our model may be realizable in artificial Rydberg atoms [18], which are condensed matter systems behaving in a Rydberg-like fashion.

Once $K(E)$ has been fixed, the bound-state energies $E$ are obtained numerically by enforcing the boundary conditions in equation (10) and then the coefficients $Z_i(E)$ are retrieved by solving the relevant linear system. While the number of bound states is infinite, good numerical convergence is obtained by taking about 200 states above and 200 states below the energy interval of interest. The metric employed in the numerical computations is thus a $400 \times 400$ matrix.

For the purpose of illustration, we will determine the weak value of the radial momentum of the excited electron and the weak value of the energy, assuming in both cases postselection can be made to a final state identical to the initial one. We choose an initial state $\left| \alpha(t=0) \right>$, which we take to be a Gaussian localized radially very far from the target, at the outer turning point of the radial potential for an excited electron (with a mean energy $n=42$), with the target being in its ground state. Initially, $\left| \alpha(t=0) \right>$ is defined on an orthogonal basis of $H_{ph}$ but we assume (and verify numerically) that this state can approximately be expanded on our chunk of computed eigenstates of $\tilde{H}$ as

$$\left| \alpha(t=0) \right> = \left| F_{loc}(r \approx r_{tp}) \right| \left| \epsilon_1 \right> = \sum a(E) \left| \psi(E) \right>,$$

where $a(E)$ are determined as in equation (20). We now proceed to compute weak values.

4.2. Weak value of the energy

We consider a scheme in which a WM of the energy is made at $t = t_W$, immediately followed by a projection to a final state. We assume for definiteness that it is possible to postselect on a state $\left| \beta_f \right>$ identical to the initial state $\left| \alpha(t=0) \right>$, e.g., by considering a WM apparatus consisting in an array of devices placed spherically at a radial distance $r \approx r_{tp}$ from the atomic core; the WM time $t_W$ must then correspond to the recurrence time (when the wavepacket relocates periodically at the turning point [19]) in the initial scattering channel, here channel 1.

If non-Hermitian issues are ignored, then the operator $H$ of equation (12) would be employed for the Hamiltonian, the evolution operator, accounting for the evolution of the system from $t = 0$ to $t_W$, would be taken as $U(t_W) = \sum_E e^{-iEt_W} \left| \psi(E) \right> \left< \psi(E) \right|$ and the weak value obtained from the usual definition (3) would thus be given by

$$\left< H(t_W) \right>_W = \frac{\left< \beta_f | H | \psi(t_W) \right>}{\left< \beta_f | \psi(t_W) \right>},$$

$$= \frac{\left< \alpha(t=0) | HU(t_W) | \alpha(t=0) \right>}{\left< \alpha(t=0) | U(t_W) | \alpha(t=0) \right>}. \quad (26)$$

This quantity is plotted in figure 1 (dotted lines) for different possible choices of the measurement time $t_W$ compatible with the system wavepacket radially localized in the neighborhood of the measuring apparatus.

However, since the system is non-Hermitian, equations (26)–(27) should formally be replaced by
The weak value of the energy (in atomic units $10^{-5}$) is shown for different measurement times compatible with the system wavepacket being in the neighborhood of the WM device. The dashed (gray, online red) line represents the usual weak value expression, given by equations (26) and (27). The solid black line represents the correct expressions equations (28) and (29) for the weak value of the energy in non-Hermitian systems. The time is given in units of the wavepacket period (about $1.15 \times 10^{-11}$ s). The average energy of the system is $-27.89 \times 10^{-5}$ au.

\[
\langle H(t_W) \rangle_W = \frac{\langle \beta_f | H | \psi(t_W) \rangle}{\langle \beta_f | \psi(t_W) \rangle},
\]

(28)

\[
= \frac{\langle \alpha(t=0) | H(t_W) | \alpha(t=0) \rangle}{\langle \alpha(t=0) | U(t_W) | \alpha(t=0) \rangle},
\]

(29)

where $\tilde{H}$ is the non-Hermitian Hamiltonian given by equation (16) and $\tilde{U}(t)$ is the corresponding evolution operator given by equation (22). This quantity is also plotted in figure 1 (solid line).

The results shown in figure 1 indicate similar overall behavior for the two curves, though there are substantial differences for several values of the measurement time\(^5\). Therefore, the replacement of the usual formulas (26)–(27) by equations (28) and (29) is not purely formal: in practical computations, the non-Hermitian nature of the system, coupled to a WM device, must be taken into account in order to compute correctly the expected shift in the pointer of the measurement apparatus due to the WM.

### 4.3. Weak value of the momentum

Another example is the weak value of the radial momentum postselected to a given position. This has become a standard example [20] involving a WM of an observable that is incompatible with the postselected one. Here, rather than postselecting to a position $|r\rangle$ known with infinite precision, we employ as above $|\beta_f\rangle = |\alpha(t=0)\rangle$ as the postselected state, keeping in mind that $\langle r | \alpha(t=0) \rangle$ is a wavefunction tightly localized around the turning point $r_{tp}$ (see equation (25)). As in the previous example we assume the WM on the preselected state can be made at different times $t_W$ for which the system wavepacket relocalizes in the neighborhood of the measuring apparatus.

The weak value (24) becomes

\[
\langle P(t_W) \rangle_W = \frac{\langle \beta_f | P | \psi(t_W) \rangle}{\langle \beta_f | \psi(t_W) \rangle},
\]

(30)

with $|\psi(t_W)\rangle = \tilde{U}(t_W)|\alpha(t=0)\rangle$. Note that $\langle P(t_W) \rangle_W$ has both a real and a complex part: the real part is related to the average velocity field of the system, while the complex part

\(^5\) Figure 1 shows the real part of the weak value—there is also an imaginary part that is several orders of magnitude smaller.
is proportional to the logarithmic derivative of the system wavefunction modulus [21]. In principle, both the real and the complex parts can be experimentally observed (though not jointly). The real part of the weak value (30) is plotted in figure 2 (black solid line). The dashed line is obtained by a straightforward application of equation (3), i.e. when the non-Hermitian character of the system is not taken into account. The two curves nearly overlap, which can appear a little surprising in view of the fact that $U(t)$ is not unitary and therefore probability is not conserved. Notwithstanding there are measurement times for which the discrepancy between equation (3) and the correct equation (24) is important.

5. Summary and conclusion

We have investigated WM for quantum systems described by a non-Hermitian Hamiltonian. The standard definition (3) of the weak value—a quantity that can in principle be experimentally observed by reading the pointer of a weak meter—does not hold in a non-Hermitian framework. The modified expression given by equation (24) was derived in this work in the context of bound-state scattering theory. The advantage of employing this particular instance of non-Hermitian formalism is that its physical meaning is devoid of any ambiguity, but equation (24) is valid for any general non-Hermitian system (provided the relevant similarity transform can be defined).

The results were illustrated numerically in a model system (a Rydberg atom with a scattering matrix having an unusually strong energy dependence) by computing the weak values of the energy and of the momentum, with a postselection to a state identical to the initial radially localized wavefunction. Overall, the results indicate that even in a non-Hermitian in which the non-diagonal elements of the metric are relatively small (the non-Hermiticity index was $\kappa = 0.061 \ll 1$), it is important in concrete studies of WM to employ the correct (i.e. non-Hermitian) formulas in order to account appropriately for the behavior of the weak meters.

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