Non-Hermitian quantum dynamics

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An algorithm previously obtained for complex-energy modal probabilities in non-Hermitian quantum dynamics is generalized to determine expectation values for arbitrary observables. When cast in conventional form, the formalism including the generalized algorithms appears as a natural generalization of conventional quantum theory, in that conventional quantum theory obtains in the continuous Hermitian limit.

I. INTRODUCTION

As shown by Weisskopf and Wigner,[1] a quantum system initially in an unperturbed, energy eigenstate, to second order in a perturbative coupling to an energy-conserving continuum, experiences effectively both a real and imaginary energy shift. This leads to simple exponential attenuation of the probability $P_N(t)$ of finding the system in the initial state for times $t>0$, i.e., after the perturbation is switched on.

In a general theorem due to Fock and Krylov,[2] any quantum state coupled to an energy-conserving continuum of states undergoes irreversible decay, in that the nondecay probability $P_N(t)\rightarrow 0$ as $t\rightarrow\infty$.

In the general case with several discrete states perturbatively coupled among themselves as well as to an energy-conserving continuum, projection-operator techniques may be employed to construct effective non-Hermitian Hamiltonians which describe the limited dynamics within the coupled, decaying subspace. This procedure has been employed in the decay theory of K mesons,[3] nuclear reaction theory,[4] optical resonator theory,[5] and in theories of multiphoton ionization and excitation.[6-8]

It turns out, however, that the correct generalization of the Weisskopf-Wigner analysis[1] to decaying, coupled quantum substates is not trivial or completely obvious. In particular, the customary construction of nonionization-nondecay probability $P_N(t)$ as a norm of the subspace state $|\Phi(t)\rangle$, i.e., $P_N(t)=\langle\Phi(t)|\Phi(t)\rangle$, has been shown to be not generally correct.[7,8]

In a detailed investigation of non-Hermitian Hamiltonians, their eigenstates and dynamics, and by requiring the finite-time definition of $P_N(t)$ to equal S-matrix results asymptotically, the present author has obtained the generally correct algorithm that utilizes the complex-energy eigenstates.[7,8]

In non-Hermitian dynamics (NHD), the statements of closure and of "sum over final-state probabilities" are formally different. The correct algorithm in non-Hermitian dynamics becomes, in the Hermitian limit, identical to the norm of state because the closure relation for the subspace appears in the "sum over final-state probabilities."[7,8]

The conclusion that non-Hermitian dynamical analyses of a decaying subspace of states coupled by a strong perturbation must employ a different, more general, algorithm has significant consequences. First, the algorithm eliminates nontrivial contributions arising from the overlap of nonorthogonal complex-energy states in the usual norm-of-state calculation. Second, one then has only independent decay from each of the complex-energy eigenmodes and, at least in the second-order calculations, this decay is simply exponential. Models of decay or ionization which employ a norm-of-state definition of $P_N(t)$ invariably show unphysical oscillations between being decayed and being nondecayed, arising because of the nonvanishing overlap of eigenstates of the non-Hermitian Hamiltonian.[6]

Not addressed in this paper is the possibility of power-law modifications to simple exponential decay[9] associated with higher-than-simple-pole singularities in the energy plane. Nor do we attempt here to define completely the exact environment in which a non-Hermitian Hamiltonian may be a realistic modeling of the physics, except to note that decays and ionizations do become objective facts with exponential regularity. An excellent review of these and related questions is available.[10] Finally, here we make no effort to analyze the influence of frequent measurements on the dynamics of an unstable system.[11] In this paper we simply accept the proven utility of effective, non-Hermitian dynamics and attempt to add some theoretical detail as it pertains to NHD in a general way.

The organization of this paper is as follows. In Sec. II we present a brief review of essential results from our previous analyses.[7,8] We present an additional argument, simple and direct, using unitarity, to infer the correct construction of intermediate-time probability $P_N(t)$ utilizing eigenstates of the adjoint Hamiltonian. In Sec. III we consider the general derivation of effective, time-dependent Schrödinger equations. We show that for t-local non-Hermitian Hamiltonians $\hat{H}(t)$ and $\hat{H}^{\dagger}(t)$ to exist, the decay-causing perturbation $V(t)$ can have only adiabatic variation. Causal transition amplitudes are constructed that are consistent with the S-matrix limit. In Sec. IV we analyze the construction of expectation values of arbitrary operators. When cast in parallel with

traditional formalism, the result appears as a nonunitary transformation on bound-space projected operators. We also obtain the generalized density matrix and its equation of motion, and generalized Ehrenfest relations. In Sec. V we make some summary remarks.

II. MODAL OCCUPATION PROBABILITIES

We review here, for convenient reference, essential conclusions of our previous NHD analysis,[7,8] and provide a further argument, from unitarity and consistency with the S matrix, for our proposed intermediate-time algorithms for modal probability.

Consider any quantum system containing both discrete, i.e., bound, states, and continuum (e.g., translational) states, the set of which we shall designate as P, plus at least one distinct class of only continuum states, which states we shall designate collectively as Q. Let the states P and Q be energy eigenstates of a Hermitian Hamiltonian H_0. We shall refer explicitly only to the discrete bound subspace of P in most of the following.

Suppose all the states P and Q are coupled by a time-dependent interaction $V(t)$, such that $V(t)$ is different from zero only for times between some initial time t_i and some future time t_f. Thus the Hamiltonian for the system is

$$H(t)=H_0+V(t) \tag{1}$$

with

$$V(t)\neq 0, \quad t_i \leq t \leq t_f \ . \tag{2}$$

We shall permit t_i and t_f to be possibly infinitely remote past and future times, so that the interaction may be constant, but generally we consider $V(t)$ to vary arbitrarily. There should be no confusion, in context, by letting the symbols P and Q also represent the respective projection operators for the subspaces, satisfying $P^2=P$, $Q^2=Q$, $PQ=QP=0$, and $P+Q=I$. The Hilbert space is thus apportioned into disjoint complements, P space and Q space.

The P-space states may correspond physically to, for example, K_0 states, excited-atom states, or atom plus photons, where the photons may ionize the atom. Thus P space comprises a set of initial states which are unstable to decays to Q space after $V(t)$ becomes nonzero. We shall refer to the system whose quantum state is in P space as an "unstable," or "decaying" system, by virtue of the Fock-Krylov theorem which informs us that eventually the system will definitely not be in P space. The system may be simply a decaying atomic state, or an arbitrarily complicated scattering complex which includes decaying states.

Q space comprises all states that are connected by $V(t)$ to P space; π-mesonic continua, atom plus emitted-photon states or ionized-atom states in the examples given. One may freely choose to associate other continua, such as those of Raman processes, leptonic modes, etc. with either P or Q. The essential point is that, for time $t=t_i$, it is a given initial condition that the quantum system is in P space. The only requirement on Q space is that it be strictly a continuum, with no disjoint discrete subspaces.

We define the total probability that the system at time t, $t_i<t<t_f$, is in P space to be $P_N(t)$, and the probability that the system is in Q space is $P_D(t)$, where we must have, by unitarity,

$$P_N(t)+P_D(t)=1 \ . \tag{3}$$

The effective, non-Hermitian Hamiltonian $H(t)$ that describes the dynamics only within P space, while also accounting for loss of probability from P space, is[8]

$$H(t)=P[H_0+V(t)-S(t)-i\Gamma(t)]P \tag{4}$$

where $S(t)$ is the Hermitian energy-shift operator and $i\Gamma(t)$ is a non-Hermitian (complex energy-shift) operator which leads to decreasing $P_N(t)$. These operators are defined in detail in Ref. 8. Here we require only their properties under Hermitian conjugation.

For the Hamiltonian (4) there exists a set of eigenvectors $\{|A_r(t)\rangle\}$, while for the adjoint $\hat{H}^\dagger(t)$ there exists an associated set of eigenvectors $\{|\overline{A}_r(t)\rangle\}$. Thus

$$\hat{H}(t)|A_r(t)\rangle=\lambda_r(t)|A_r(t)\rangle \tag{5}$$

and

$$\hat{H}^\dagger(t)|\overline{A}_r(t)\rangle=\lambda_r^*(t)|\overline{A}_r(t)\rangle \ . \tag{6}$$

With normalization these two sets of eigenvectors will constitute biorthogonal sets[12,8] in that

$$\langle A_r(t)|\overline{A}_s(t)\rangle=\langle \overline{A}_s(t)|A_r(t)\rangle^*=\delta_{r,s} \tag{7}$$

and the completeness relation on P space may be expressed as

$$\sum_r |A_r(t)\rangle\langle \overline{A}(t)|=I \ . \tag{8}$$

As has been shown,[7,8] the states $|A_r(t)\rangle$ and $|\overline{A}_r(t)\rangle$ are P-space projected Lippmann-Schwinger states satisfying, respectively, "incoming" and "outgoing" boundary conditions. (Recall that, even though we are interested primarily in the dynamics within the discrete, bound states of P space, these are embedded in at least an underlying translational continuum which permits the manipulation of the necessary distributions in the derivation of this result.) Because $V(t_i)=V(t_f)=0$, we have

$$\lim_{t\to t_{i,f}} |A_r(t)\rangle=|a_r\rangle \ , \tag{9}$$

$$\lim_{t\to t_{i,f}} |\overline{A}_r(t)\rangle=|a_r\rangle \ , \tag{10}$$

where the noninteracting ("undressed") states $|a_r(t)\rangle$ satisfy

$$H_0|a_r\rangle=\varepsilon_r|a_r\rangle \ , \tag{11}$$

a real-eigenvalue equation for the Hermitian H_0.

We shall provisionally associate to the statement, for $t>t_i$, "a system is in an $\hat{H}$ eigenstate $|A_r(t)\rangle$" the implication that the system has not decayed or ionized, has an energy $\mathrm{Re}\lambda_r(t)$, and has a probability of decaying or ion-

izing equal to $-2\,\mathrm{Im}\lambda_r(t)$ per unit of time. (Of course, the latter can be justified operationally only over an ensemble of similar systems.)

The amplitude $S_{s,r}$ that, given the system at t_0 is in the state $|A_r(t_0)\rangle$, at some time $t>t_0$ the system will be found in the $\hat{H}$ eigenstate $|A_s(t)\rangle$, is given by the expression[8]

$$S_{s,r}=\langle \overline{A}_s(t)|\phi_r(t)\rangle \tag{12}$$

where the state $|\phi_r(t)\rangle$ is obtained from solving the Schrödinger equation

$$H(t)|\phi_r(t)\rangle=i\frac{d}{dt}|\phi_r(t)\rangle\ , \tag{13}$$

subject to the initial condition

$$\lim_{t\to t_0}|\phi_r(t)\rangle=|A_r(t_0)\rangle\ .$$

The corresponding probability that the system at time $t>t_0$ is in the eigenstate $|A_s(t)\rangle$ is

$$P_{s,r}(t)=|S_{s,r}|^2=\langle\phi_r(t)|\overline{A}_s(t)\rangle\langle\overline{A}_s(t)|\phi_r(t)\rangle\ . \tag{14}$$

More generally, we may permit the system to be in an arbitrary P-space state $|\phi_i(t_0)\rangle$ at time t_0, which, by the completeness Eq. (8), we may express as

$$|\phi_i(t_0)\rangle=\sum_r c_r(t_0)|A_r(t_0)\rangle\ . \tag{15}$$

The amplitude $S_{s,i}$ for finding the system in eigenstate $|A_s(t)\rangle$ at time $t>t_0$ is then

$$S_{s,i}=\langle\overline{A}_s(t)|\phi_i(t)\rangle \tag{16}$$

and the corresponding probability is

$$P_{s,i}(t)=|S_{s,i}|^2=\langle\phi_i(t)|\overline{A}_s(t)\rangle\langle\overline{A}_s(t)\rangle\langle\overline{A}_s(t)|\phi_i(t)\rangle\ . \tag{17}$$

Finally, the total P-space probability at intermediate times is obtained by summing $P_{s,i}(t)$ over all possible ("final") states $|\overline{A}_s(t)\rangle$, which gives

$$\begin{aligned}P_N(t)&=\sum_s|S_{s,r}|^2\\&=\sum_s\langle\phi_i(t)|\overline{A}_s(t)\rangle\langle\overline{A}_s(t)|\phi_i(t)\rangle\ .\end{aligned} \tag{18}$$

Note that this result requires the particular initial normalization condition on the expansion coefficients

$$\begin{aligned}P_N(t_0)&=\sum_s\langle\phi_i(t_0)|\overline{A}_s(t_0)\rangle\langle\overline{A}_s(t_0)|\phi_i(t_0)\rangle\\&=\sum_r|c_r(t_0)|^2=1\ ,\end{aligned} \tag{19}$$

a condition that is quite different from the traditional requirement[3]

$$\langle\phi_i(t_0)|\phi_i(t_0)\rangle=1\ , \tag{20}$$

because of the nonorthogonality of the eigenstates $|A_s(t)\rangle$.

The constructions (12)–(18) are consistent with the asymptotic, S-matrix limit.[8] That is, for $t_i\to-\infty$, $t_f\to\infty$, recall that the formalism we are using applies for an arbitrary assemblage of decaying, scattering and/or ionizing systems. Our constructions thus include the correct composition of "incoming waves in outgoing states," etc.[13] reproducing thereby the overall S-matrix results.

We can, however, present a more direct approach using unitarity. Consider an adiabatic, but otherwise arbitrary, interaction with a non-Hermitian Hamiltonian such as (4). Let the initial state at $t\to-\infty$ be

$$|\phi_i(-\infty)\rangle=\sum_r c_r|a_r\rangle\ . \tag{21}$$

The calculation of $P_N(\infty)$ leads to[7,8]

$$P_N(\infty)=\sum_r|c_r|^2\exp\left[-\int_{-\infty}^{\infty}\gamma_r(t)dt\right]\ . \tag{22}$$

Now, writing

$$\begin{aligned}&\exp\left[-\int_{-\infty}^{\infty}\gamma_r(t)dt\right]\\&\quad=1-\int_{-\infty}^{\infty}\gamma_r(t)dt\exp\left[-\int_{-\infty}^{t}\gamma_r(t')dt'\right]\end{aligned} \tag{23}$$

for each term in (22), we have

$$\begin{aligned}&P_N(\infty)\\&\quad=\sum_r|c_r|^2\left[1-\int_{-\infty}^{\infty}\gamma_r(t)dt\exp\left[-\int_{-\infty}^{t}\gamma_r(t')dt'\right]\right]\end{aligned} \tag{24}$$

$$=1-\sum_r|c_r|^2\int_{-\infty}^{\infty}\gamma_r(t)dt\exp\left[-\int_{-\infty}^{t}\gamma_r(t')dt'\right] \tag{25}$$

where we have used normalization of the initial state, $\sum_r|c_r|^2=1$. Recalling the unitarity condition (3), we therefore obtain

$$\begin{aligned}P_D(\infty)=&\sum_r|c_r|^2\\&\times\int_{-\infty}^{\infty}\gamma_r(t)dt\exp\left[-\int_{-\infty}^{t}\gamma_r(t')dt'\right]\ ,\end{aligned} \tag{26}$$

so that we may identify, or in any case *assign*, independent modal occupation probabilities,

$$P_r(t)=|c_r|^2\exp\left[-\int_{-\infty}^{t}\gamma_r(t')dt'\right]\ . \tag{27}$$

Then

$$P_D(\infty)=\sum_r|c_r|^2\int_{-\infty}^{\infty}\gamma_r(t)P_r(t)dt\ , \tag{28}$$

as one would expect consistently with previous results.[7,8] The finite-time amplitude construction (12), and the modal probability construction (14), are therefore dictated unambiguously by unitarity and consistency with the S-matrix limit.

It is noteworthy that the lack of oscillations in $P_N(t)$,

because of (3), is equivalent to no oscillations in $P_D(t)$. That there are no oscillations is $P_D(t)$, that is, no quantum beats in the *total* decay amplitude, is well known.[4]

III. TIME-DEPENDENT EFFECTIVE SCHRÖDINGER EQUATIONS

Here we analyze conditions under which a non-Hermitian Schrödinger equation such as (13) may obtain as a local-time effective Hamiltonian. For the Hermitian Hamiltonian (1), the exact dynamical evolution of the system is described by the familiar Schrödinger equation,

$$H(t)|\Psi(t)\rangle = \frac{id}{dt}|\Psi(t)\rangle \tag{29}$$

with H as defined in (1).

We apportion the Hilbert space, using the projection operators P and Q defined above, by applying them to Eq. (29) to find

$$(H_{\rm opp}+V_{pp})P|\Psi(t)\rangle + V_{pq}Q|\Psi(t)\rangle = \frac{id}{dt}P|\Psi(t)\rangle \ , \tag{30}$$

and

$$(H_{0qq}+V_{qq})P|\Psi(t)\rangle + V_{qp}P|\Psi(t)\rangle = \frac{id}{dt}Q|\Psi(t)\rangle \ , \tag{31}$$

where $V_{pq}=PVQ$, etc. Letting $P|\Psi(t)\rangle = |\Psi_p(t)\rangle$ and $Q|\Psi(t)\rangle = |\Psi_q(t)\rangle$, and ignoring the rescattering term V_{qq}, which is irrelevant for present considerations, we have the resulting Schrödinger equation for $|\Psi_q\rangle$:

$$\left[\frac{id}{dt}-H_{0qq}\right]|\Psi_q\rangle = V_{qp}|\Psi_p\rangle \ . \tag{32}$$

We define a retarded Green function

$$\left[\frac{id}{dt}-H_{0qq}+i\epsilon\right]G^R_{qq}(t-t') = Q\delta(t-t') \ , \tag{33}$$

and an advanced Green function

$$\left[\frac{id}{dt}-H_{0qq}-i\epsilon\right]G^A_{qq}(t-t') = Q\delta(t-t') \ . \tag{34}$$

It is understood that the limit $\epsilon\to 0+$. Formal solutions to (33) and (34) are readily obtained:

$$G^R_{qq}(t-t') = \frac{Q}{2\pi}\int d\omega \frac{1}{\omega - H_{0qq}+i\epsilon}\exp[-i\omega(t-t')] \ , \tag{35}$$

and

$$G^A_{qq}(t-t') = \frac{Q}{2\pi}\int d\omega \frac{1}{\omega - H_{0qq}-i\epsilon}\exp[-i\omega(t-t')] \ . \tag{36}$$

One typically is interested in initial conditions corresponding to probability unity for having an unstable system. This corresponds to setting $|\Psi_q(t_i)\rangle_+ = Q|\Psi(t_i)\rangle = 0$.

We can now construct transition amplitudes *within P* space. This requires a future state with a "final-state" condition $(\Psi_q(t_f)\rangle_- = Q|\Psi(t_f)\rangle = 0$. To solve for *P-P* transitions only, we employ (35) and (36) to obtain the corresponding retarded and advanced solutions satisfying $|\Psi_q(t_i)\rangle_+ = |\Psi_q(t_f)\rangle_- = 0$:

$t \ge t_i$;

$$|\Psi_q(t)\rangle_+ = \int G^R_{qq}(t-t')V_{qp}(t')|\Psi_p(t)\rangle_+ dt' \tag{37}$$

and

$t \le t_f$;

$$|\Psi_q(t)\rangle_- = \int G^A_{qq}(t-t')V_{qp}(t')|\Psi_p(t)\rangle_- dt' \ . \tag{38}$$

These may be employed in the corresponding retarded and advanced versions of the left-hand sides of (30):

$$[H_{0pp}+V_{pp}(t)]|\Psi_p(t)\rangle_+ + V_{pq}(t)\int G^R_{qq}(t-t')V_{qp}(t')|\Psi_p(t')\rangle_+ dt' \tag{39}$$

and

$$[H_{0pp}+V_{pp}(t)]|\Psi_p(t)\rangle_- + V_{pq}(t)\int G^A_{qq}(t-t')V_{qp}(t')|\Psi_p(t')\rangle_- dt' \ . \tag{40}$$

We identify two effective-Hamiltonian operators, nonlocal in time,

$$H_\pm|\Psi_p(t)\rangle_\pm = [H_{0pp}+V_{pp}(t)]|\Psi_p(t)\rangle_\pm + V_{pq}(t)\int G^{R,A}_{qq}(t-t') \times V_{qp}(t')|\Psi_p(t')\rangle_\pm dt' \ . \tag{41}$$

Thus far we have made no approximation. Equations (39) and (40) account fully for the exact P-space component of the state vector, allowing for regeneration of P-space states through $Q\to P$ transitions as well as for direct P-space transitions. However, no further general step may be taken without approximation of some kind.

The first restricting assumption we consider is that of adiabatic modulation of the interaction $V(t)$. We write $V(t)$ in the form

$$V(t) = \eta(t)V(0) \ , \tag{42}$$

where adiabatic modulation requires the Fourier transform of $\eta(t)$ to approximate a δ function:

$$\eta(k) = \int \eta(t)\exp(ikt)dt \approx \delta(k) \ . \tag{43}$$

Substituting (43) into (41), and use of (35)–(38), leads to

$$H_{\pm}|\Psi_p(t)\rangle_{\pm}=[H_{0pp}+V_{pp}(t)]|\Psi_p(t)\rangle_{\pm}+V_{pq}(t)\frac{Q}{2\pi}\int dt'\int d\omega\frac{1}{\omega-H_{0qq}\pm i\epsilon}\exp[-i\omega(t-t')]$$
$$\times\int dk\exp(-ikt')\eta(k)V_{qp}(t')|\Psi_p(t')\rangle_{\pm}\ . \tag{44}$$

We now consider the traditional[1] approximation to second order in V_{qp}, letting

$$|\Psi_p(t')\rangle\approx\exp(-iH_{0pp}t')|\Psi_p(0)\rangle\ . \tag{45}$$

We may represent the projection operator Q as

$$Q=\int de|e\rangle\langle e| \tag{46}$$

where the states $|e\rangle$ are eigenstates of H_0:

$$H_0|e\rangle=e|e\rangle\ . \tag{47}$$

With (44), (45), and (46) we easily perform the integrations to obtain

$$H_{\pm}=H_{0pp}+V_{pp}(t)$$
$$+V_{pq}(t)\int de|e\rangle\langle e|V_{ep}(t)\frac{1}{e-H_{0pp}\pm i\epsilon}\ , \tag{48}$$

which are now t-local operators. Further, letting

$$\hat{H}(t)=H_{+}(t) \tag{49}$$

we have that

$$\hat{H}^{\dagger}(t)=H_{-}(t)\ . \tag{50}$$

Thus Eqs. (30) and (31) become, for P-space amplitudes satisfying, respectively, initial- and final-state conditions $\Psi_q(t_i)\rangle_{+}=|\Psi_q(t_f)\rangle_{-}=0$,

$$\hat{H}(t)|\Psi_p(t)\rangle_{+}=\frac{id}{dt}|\Psi_p(t)\rangle_{+} \tag{51}$$

and

$$\hat{H}^{\dagger}(t)|\Psi_p(t)\rangle_{-}=\frac{id}{dt}|\Psi_p(t)\rangle_{-}\ . \tag{52}$$

Using in (48) the familiar relation

$$\int dx\frac{1}{x\pm i\epsilon}=\mathrm{P}dx\frac{1}{x}\mp i\pi\delta(x)\ , \tag{53}$$

where P denotes principal value integration, we finally obtain explicit expressions for the operators $S(t)$ and $\Gamma(t)$ in Eq. (4):

$$S(t)=V_{pq}(t)\int de|e\rangle\langle e|V_{pq}(t)\frac{1}{H_{0pp}-e} \tag{54}$$

and

$$\Gamma(t)=\pi V_{pq}(t)\int de|e\rangle\langle e|V_{pq}(t)\delta(H_{0pp}-e)\ , \tag{55}$$

the same results as Eqs. (25) and (26), and (54) and (55) in Ref. 8.

Equations (51) and (52) determine the time evolution of the P-space component of state vectors subject to prescribed initial and final conditions. Causality dictates that the retarded states evolve under $\hat{H}$, whereas the advanced states retroevolve under $\hat{H}^{\dagger}$. Moreover, it is only in the limit of adiabatic modulation of $V(t)$ that the dynamics is local in time.

The same causal considerations which led to Eqs. (51) and (52) also dictate the construction of transition amplitudes. In particular, given an initial P state $|\Psi_p^i(t_i)\rangle$ at time t_i, the amplitude for a transition to a particular P state $|\Psi_p^f(t_f)\rangle$ at time t_i is

$$S_{f,i}(t_f,t_i)=-\langle\Psi_p^f(t_f)|\Psi_p^i(t_i)\rangle_{+} \tag{56}$$

where t is any time between t_i and t_f, and the states $|\Psi_p^i(t_i)\rangle_{+}$ and $|\Psi_p^f(t_f)\rangle_{-}$ satisfy (51) and (52), respectively, subject to the initial- and final-state conditions

$$\lim_{t\to t_i}|\Psi_p^i(t)\rangle_{+}=|\Psi_p^i(t_i)\rangle \tag{57}$$

and

$$\lim_{t\to t_f}|\Psi_p^f(t)\rangle_{-}=|\Psi_p^f(t_f)\rangle\ . \tag{58}$$

In order to have a notation specifically for the context of NHD, we define

$$|\Phi_i(t)\rangle=|\Psi_p^i(t)\rangle_{+} \tag{59}$$

and

$$|\overline{\Phi}_f(t)\rangle=|\Psi_p^f(t)\rangle_{-} \tag{60}$$

so that (56) takes the form

$$S_{f,i}(t_f,t_i)=\langle\overline{\Phi}_f(t)|\Phi_i(t)\rangle\ , \tag{61}$$

the same as (59) in Ref. 8.

IV. OPERATOR EXPECTATION VALUES

Given a bound-subspace state $|\Phi(t)\rangle$ for a decaying system, which evolves under a non-Hermitian Hamiltonian $\hat{H}$, the expression (17) provides the probability that the system is in the $\hat{H}$ eigenstate $|A_s(t)\rangle$. We define nonunitary transform operators $\Omega(t)$ and $\overline{\Omega}(t)$ in the P subspace such that

$$\Omega(t)|a_s\rangle=|A_s(t)\ , \tag{62}$$

and

$$\overline{\Omega}(t)|a_s\rangle=|\overline{A}_s(t)\ . \tag{63}$$

[Compare with (121) and (122) in Ref. 8.] The expression (17) may then be written in the form

$$P_{s,i}(t)=\langle\Phi_i(t)|\overline{\Omega}(t)|a_s\rangle\langle a_s|\overline{\Omega}^{\dagger}(t)|\Phi_i(t)\rangle \tag{64}$$
$$=\langle\Phi_i(t)|\hat{P}_s|\Phi_i(t)\rangle\ , \tag{65}$$

where $\hat{P}_s(t)$ is the transformed projection operator

$$\hat{P}_s(t)=\overline{\Omega}(t)|a_s\rangle\langle a_s|\overline{\Omega}^{\dagger}(t) \tag{66}$$

$$=\overline{\Omega}(T)P_s\overline{\Omega}^{+}(t)\ . \tag{67}$$

A. Operators

The expression (65) is in the conventional form of an expectation value in traditional quantum formalism. Note, however, the appropriate projection operator is related to that for the state $|a_s\rangle$ by the nonunitary transformation $\overline{\Omega}(t)$.

Imagine now that at $t=0$ the system is filtered to remove any decay products, that is, a (decaying) P-space state $|\Phi_i(0)\rangle$ is produced by measurement. At some future time t another measurement is performed upon remaining P-state systems, to determine the value of some operator (observable) O. Suppose that the value o_j is found, which value is associated with some eigenstate $|o_j\rangle$ of O. In the general case, the operator O will have nonvanishing matrix elements between Q space and P space, and the state $|o_j\rangle$ will have components in both spaces.

The amplitude to find eigenvalue o_j (conditional upon finding an undecayed system) $A(o_j)$ is obtained by causal analysis parallel to that leading to (16). We find

$$A(o_j)=\langle o_j|P\overline{\Omega}^{\dagger}(t)|\Phi_i(t)\rangle \tag{68}$$

so that the corresponding probability is

$$P(o_j)=|A(o_j)|^2$$

$$=\langle\Phi_i(t)|\overline{\Omega}(t)P|o_j\rangle\langle o_j|P\overline{\Omega}^{\dagger}(t)|\Phi_i(t)\rangle\ . \tag{69}$$

The conditional expectation value is, therefore

$$\langle\hat{O}(t)\rangle=\sum_{\{o_j\}}o_jP(o_j)=\langle\Phi_i(t)|\hat{O}(t)|\Phi_i(t)\rangle\ , \tag{70}$$

where we have defined

$$\hat{O}(t)\equiv\overline{\Omega}(t)POP\overline{\Omega}^{\dagger}(t)\ . \tag{71}$$

The sum in (70) is over the entire spectrum of the operator O.

The expression (71) is the generalization of the result in (67). If one expresses expectation values in the conventional form (70), causal analysis requires the operators must be transformed according to (71).

Note that a transformed Hamiltonian could be also defined according to (71). It is not, however, a particularly useful definition. The Hamiltonians that determine the time evolution of the unstable, decaying system are defined in Eqs. (48)–(50). We shall continue to use the notation $\hat{H}$ and $\hat{H}^{\dagger}$ for the "given" non-Hermitian Hamiltonians, whereas all other effective operators must be transformed as prescribed in (71).

In general, it would be difficult to construct the explicit solutions for the transformation operator $\Omega(t)$. In the requisite adiabatic limit, however, such as obtains especially for ordinary mesonic decays or multiphoton ionization, the general solution is readily obtained. It is provided in (122) of Ref. 8, which for completeness we restate here:

$$\Omega(t)=(|A_1(t)\rangle,|A_2(t)\rangle,|A_3(t)\rangle,\ldots) \tag{72}$$

where $|A_i(t)\rangle$ is an eigenket in columnar form.

B. Density matrix

We may allow for the possibility that the system is not in a pure P state $|\Phi_i(t)\rangle$, but rather is in a mixture of such states with corresponding classical probabilities P_i. Allowing for this, the result (70) generalizes to

$$\langle\hat{O}(t)\rangle=\sum_{\{i\}}P_i\langle\Phi_i(t)|\hat{O}(t)|\Phi_i(t)\rangle \tag{73}$$

where the sum in (73) is over all states i in P space. Expanding $|\Phi_i(t)\rangle$ in the basis set $\{|A_s(t)\rangle\}$ using (7) we obtain

$$|\Phi_i(t)\rangle=\sum_{\{i\}}\langle\overline{A}_s(t)|\Phi_i(t)\rangle|A_s(t)\rangle\ . \tag{74}$$

The expression (73) then may be rewritten as

$$\langle\hat{O}(t)\rangle=\sum_{\{i,r,s\}}P_i\langle\overline{A}_s(t)|\Phi_i(t)\rangle^*\langle A_s(t)|\hat{O}(t)|A_r(t)\rangle\langle\overline{A}_r(t)|\Phi_i(t)\rangle$$

$$=\sum_{\{i,r,s\}}P_i\langle\overline{A}_r(t)|\Phi_i(t)\rangle\langle\Phi_i(t)|\overline{A}_s(t)\rangle\langle A_s(t)|O(t)|A_r(t)\rangle$$

$$=\sum_{\{r\}}\langle\overline{A}_r(t)|\hat{\rho}(t)\hat{O}(t)|A_r(t)\rangle \tag{75}$$

where we have defined a density matrix $\rho(t)$ as

$$\hat{\rho}(t)=\sum_{\{i\}}P_i|\Phi_i(t)\rangle\langle\Phi_i(t)|\ . \tag{76}$$

Finally, if we define a trace operator Tr* such that

$$\mathrm{Tr}^*\hat{\rho}(t)\hat{O}(t)=\sum_{\{r\}}\langle\overline{A}_r(t)|\hat{\rho}(t)\hat{O}(t)|A_r(t)\rangle\ , \tag{77}$$

then we obtain the general expression

$$\langle\hat{O}(t)\rangle=\mathrm{Tr}^*\hat{\rho}(t)\hat{O}(t)\ . \tag{78}$$

The equation of motion of the generalized (adiabatic) density matrix is readily obtained using (51);

$$\dot{\hat{\rho}}(t)=\frac{d\hat{\rho}(t)}{dt}=\frac{d}{dt}\sum_{\{i\}}P_i|\Phi_i(t)\rangle\langle\Phi_I(t)| \tag{79}$$

$$=-i\hat{H}(t)\hat{\rho}(t)+i\hat{\rho}(t)\hat{H}^{\dagger}(t) \tag{80}$$

or

$$\frac{id\hat{\rho}(t)}{dt}=[\hat{H}(t),\hat{\rho}(t)]+\hat{\rho}(t)[\hat{H}(t)-\hat{H}^{\dagger}(t)]\ . \tag{81}$$

It is helpful in understanding the preceding results to consider them in the adiabatic limit. In the adiabatic limit we have [Eq. (92) in Ref. 8], for any initial P state at time t_0,

$$|\Phi_i(t)\rangle=\sum_{\{r\}}C_r^i(t_0)\exp\left[-i\int_{t_0}^{t}\lambda_r(t')dt'\right]|A_r(t)\rangle\ . \tag{82}$$

Defining matrix elements as, for example,

$$\hat{\rho}_{r,s}(t)=\langle\overline{A}_r(t)|\hat{\rho}(t)|\overline{A}_s(t)\rangle\ , \tag{83}$$

and taking time derivatives directly using (68), (74), and (81) in Ref. 8, we find in the adiabatic limit

$$i\dot{\hat{\rho}}_{r,s}(t)=\sum_{\{n\}}[\hat{H}_{r,n}(t)\hat{\rho}_{n,s}(t)-\hat{\rho}_{r,n}(t)\hat{H}^{\dagger}_{n,s}(t)] \tag{84}$$

$$=\lambda_r(t)\hat{\rho}_{r,s}(t)-\hat{\rho}_{r,s}(t)\lambda_s^*(t) \tag{85}$$

$$=[\varepsilon_r(t)-\varepsilon_s(t)]\hat{\rho}_{r,s}(t)-i(\gamma_r-\gamma_s)\hat{\rho}_{r,s}(t)/2 \tag{86}$$

$$=\Delta_{r,s}(t)\hat{\rho}_{r,s}(t)-i\gamma_{r,s}(t)\hat{\rho}_{r,s}(t)\ . \tag{87}$$

We have let $\varepsilon_r(t)=\mathrm{Re}\lambda_r(t)$ and $\gamma_r=-2\,\mathrm{Im}\lambda_r(t)$ in going from (85) to (86).

Finally, it is of interest to consider (78) in the adiabatic limit. Using (71), (72), and (82) we have

$$\langle\hat{O}(t)\rangle=\sum_{\{i,r,s\}}p_iC_r^i(t_0)C_s^{*i}(t_0)O_{s,r}(t)\times\exp\left[-i\int_{t_0}^{t}[\lambda_r(t')-\lambda_s^*(t')]dt'\right] \tag{88}$$

where here

$$\hat{O}_{s,r}(t)\equiv\langle A_s(t)|\hat{O}(t)|A_r(t)\rangle \tag{89}$$

$$=\langle a_s|O(t)|a_r\rangle\ . \tag{90}$$

For example, if we set $\hat{O}(t)=\hat{H}(t)$, (87) reduces to the satisfying result

$$\langle\hat{H}(t)\rangle=\sum_{\{i,r\}}P_i|C_r^i(t_0)|^2\lambda_r(t)\exp\left[-\int_{t_0}^{t}\gamma_r(t')dt'\right]\ . \tag{91}$$

Finally, if we choose $\hat{O}$ to be the P-space identity operator, transformed according to (71), we obtain

$$\langle\hat{I}\rangle=\sum_{\{i,r\}}P_i|C_r^i(t_0)|^2\exp\left[-\int_{t_0}^{t}\gamma_r(t')dt'\right]\ , \tag{92}$$

which gives the nondecay probability at time t. For an initial pure state this becomes equivalent to the more restricted result (91) in Ref. (8).

C. Ehrenfest relations

Having obtained a generalized non-Hermitian formalism, it is appropriate to ask about the time development as usually expressed in the Ehrenfest relations. It is a simple matter to compute directly the time derivative of the effective operator defined in (71). Using (51) we readily obtain the results

$$-\frac{id}{dt}\langle\hat{O}(t)\rangle=\langle[\hat{H}(t),\hat{O}(t)]\rangle+\langle(\hat{H}^{\dagger}(t)-\hat{H}(t)]\hat{O}(t)\rangle-i\left\langle\frac{d}{dt}[\hat{O}(t)]\right\rangle\ . \tag{93}$$

In the adiabatic limit, using approximate orthogonality [Eq. (80) in Ref. 8] and the general adiabatic state (82), we find

$$-\frac{id}{dt}\langle\hat{O}(t)\rangle=\sum_{\{i,r,s\}}P_iC_r^i(t_0)C_s^{*i}(t_0)\hat{O}_{s,r}(t)(\lambda_s^*-\lambda_r)\exp\left[-i\int_{t_0}^{t}[\lambda_r(t')-\lambda_s^*(t')]dt'\right]-\left\langle\frac{d}{dt}[\hat{O}(t)]\right\rangle \tag{94}$$

where

$$\left\langle\frac{d}{dt}[O(t)]\right\rangle=\sum_{\{i,r,s\}}P_iC_r^i(t_0)C_s^{*i}(t_0)\frac{dQ_{s,r}(t)}{dt}\exp\left[-i\int_{t_0}^{t}[\lambda_r(t')-\lambda_s^*(t')]dt'\right] \tag{95}$$

and

$$O_{s,r}(t)=\langle a_s|O(t)|a_r\rangle\ . \tag{96}$$

The decay attenuation of expectation values of O in P space is thus seen to be implied in (93), and manifest in (95).

V. SUMMARY AND CONCLUSIONS

In Ref. 8 we concluded that for effectively non-Hermitian dynamical systems, transition amplitudes should be calculated by a generalized algorithm which becomes equivalent to the conventional one whenever non-Hermitian parts of the Hamiltonian vanish. This algorithm is most conveniently implemented using eigenstates of the adjoint Hamiltonian $\hat{H}^{\dagger}$. This conclusion was arrived at through a consistency requirement, that any candidate algorithm for intermediate times must asymptotically be equivalent to an S-matrix prediction. The theoretical basis for the NHD algorithm lies in a unique feature of the eigenstates of $\hat{H}^{\dagger}$, that of being projections of relevant Lippmann-Schwinger "outgoing"

states, while the eigenstates of $\hat{H}$ are projections of "incoming" states.

In the present paper we have analyzed the evolution of states according to causality requirements in the local-time limit. We have seen that the local-time limit requires that the interaction vary only adiabatically. Further, our conclusion pertaining to the correct probability algorithm in NHD follows from the correct utilization of advanced and retarded solutions to Schrödinger's equation, with proper regard for initial- and final-state boundary conditions.

We have supplied an additional argument for the general probability algorithm using both unitarity and the asymptotic S matrix. This argument shows that the algorithm leads to results for modal occupation probabilities which in any case could be reasonably assigned.

We have also extended the basic probability algorithm to the calculations of expectation values for arbitrary operators, and have developed an appropriate generalized density-matrix formalism. Although our calculations have been based upon the traditional second-order approximation,[1] it seems reasonable that our results might apply for effective, local-time non-Hermitian interactions generally. That is, our formal conclusions may be more generally relevant than the approximation in which they are inferred. In any case they provide a consistent, self-contained non-Hermitian, quantum-dynamical formalism.

As a generalization of Hermitian quantum dynamics, the formalism presented here has not only practical relevance as a generalization of Weisskopf-Wigner theory to strongly coupled decaying discrete subspaces, but also provides an interesting theoretical system for further investigations. Let us finally note that this formalism may find utility in a variety of other contexts, including the optical model in nuclear physics and, perhaps, even quantum measurement theory, which considerations we plan to address elsewhere.

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