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Non-Hermitian quantum theory of multiphoton ionization

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The construction of physical occupation and transition probabilities in non-Hermitian, effective-Hamiltonian models of coupled near-resonant discrete states which decay to a continuum is analyzed. We consider for definiteness the particular physical example of atomic multiphoton ionization. The possibility of finite duration and arbitrary modulation of this interaction, and of the subsequent ionization and/or decay, in such a system allows us to invoke "adiabatic switching" considerations in conventional S-matrix theory. The effective Hamiltonian $\hat{H}(t)$ is derived for both stationary and time-dependent Schrödinger equations. These derivations yield the same effective $\hat{H}(t)$, and further reveal that this operator is associated with discrete-state-projected "incoming" scattering states. The Hermitian conjugate operator $\hat{H}^{\dagger}(t)$ is similarly shown to be associated with discrete-state "outgoing" scattering states. This shows that effective-Hamiltonian theories are intrinsically S-matrix theories. This fact, in turn, is employed to construct transition amplitudes. The possibility of resonance in the atom-field interaction requires that both the projected incoming states and projected outgoing states be employed in this construction. The projected incoming and outgoing states in the (discrete) bound space are quite conveniently described by effective time-dependent Schrödinger equations, supplemented by initial- and final-state boundary conditions. The fact of independent-exponential decay from each mode throughout the history of the interaction, for an arbitrary initial superposition state, in the adiabatic limit, suggests a practical construction for intermediate-time bound-state probabilities. This construction permits the formal definition of individual-state probabilities, which satisfy a generalized adiabatic theorem, and leads to the satisfying result that the total bound-state probability at all intermediate times is the sum of complex-mode probabilities. In marked contrast to the conventional norm-of-state definition of nonionization probability, this sum does not have oscillations at intermediate times, in the limit of adiabatic modulation of the interaction. Superposition-state probabilities, however, exhibit oscillations at intermediate times. The resulting non-Hermitian quantum dynamics is especially suited, and even essential, for an accurate description of near-resonance ionization. Precise matching of the time-dependent $\hat{H}(t)$ and $\hat{H}^{\dagger}(t)$ with bases of their instantaneous eigenstates is required by approximate unitarity in the discrete decaying space, for a consistent theory. We illustrate these considerations in a general way in the context of resolvent-operator techniques. The implementation of the theory in both its time-dependent and stationary-state formulations is presented in an Appendix, for the completely general two-state non-Hermitian Hamiltonian. The results of these formulations are found to agree, in the adiabatic limit, to all orders in the non-Hermitian interaction. The utility of direct diagonalization of the effective $\hat{H}(t)$, advocated by Armstrong and Baker, is transparent. The overall context of interpretation of their earlier work is, however, significantly altered. Similar considerations apply for nonswitchable interactions, such as for K-meson decays. These results represent a practical generalization of quantum mechanics to non-Hermitian systems. The utility, and the necessity, of such a generalization has considerable theoretical interest, and direct experimental implications.

I. INTRODUCTION

The analysis of the ionization of bound-state systems ("atoms") through interaction with an intense electromagnetic field is made challenging through the possibility of multiphoton resonances in intermediate bound-bound transitions. Under certain circumstances, such as when the rise time and fall time of the ionizing pulse is long relative to the response of the atom, and short in duration relative to such phase-shifting processes as spontaneous emission of a photon by the atom, a Hamiltonian analysis with the time-dependent Schrödinger equation may be useful. However, it is too difficult a problem to solve exactly for the dynamic wave function for the ionizing atom-photon system. Close to resonance, low-order perturbation theory is not valid. One may attempt to perform infinite summations,[1] or take recourse to numerical studies for particular systems.[2] It is highly desirable, nonetheless, from a conceptual standpoint to construct simplified models which incorporate essential dynamical features of the actual physical situation, and which may be solved analytically in various limiting regimes of the dynamical parameters. One may thereby better understand how various features, such as ionization rates,

fluorescence, widths, etc., behave in the different regimes of intensity, detuning, and other parameters.

The simplest of the models which can include bound-bound transitions to all orders in some fashion, and also account for ionization dynamics, are two-state models with effective "decay" (to the photoelectron continuum) terms in a non-Hermitian Hamiltonian.[3] An alternative analysis employs a noninteracting "dressed-atom" basis, with eigenstates of the near-resonant atom-photon system.[4] In this approach, one should in practice evaluate cascade effects and also properly symmetrize.[5] There are nonetheless a variety of circumstances where performing the dressing is useful.[6]

Even aside from the question of practicability, however, noninteracting dressed states are not a wholly satisfactory basis. When the atom-field interaction is considered, these noninteracting dressed bases lead to predictions of ac Stark splitting of the photoelectron spectrum in conjunction with saturation of the intermediate-resonance transitions.[7] Further, this photoelectron spectrum is sensitive to the time dependence of the evolution of the atom-field interaction.[8] And finally, these states are coupled dynamically, through virtual transitions to the photoelectron continuum, and thus are not dynamically independent even to second order in the atom-field interaction, the same order to which ionization is calculated.[9]

The relatively simple non-Hermitian two-state models represent a significant step toward possible systematic inclusion of the off-diagonal interaction[9] through the continuum simultaneously with interaction time-profile effects on final-state photoelectron spectra.[8] One of the best known of such models, that of Beers and Armstrong,[3] utilizes the resolvent for the effective Hamiltonian $\hat{H}$. This formulation of the problem in effect assumes the effective atom-field interaction $\hat{H}_{\mathrm{AF}}$ is suddenly switched on, with the atom initially in an eigenstate of the noninteracting atom-field Hamiltonian H_0. Because the eigenstates of H_0 are not eigenstates of $\hat{H}$, the bound-state (nonionization) probability $P_B(t)$ exhibits temporal oscillations. This follows directly in consequence of the norm-of-state prescription $P_B(t)=\langle\phi_A(t)\,|\,\phi_A(t)\rangle$, where $|\,\phi_A(t)\rangle$ is the bound-state wave function as determined by the resolvent for $\hat{H}$.

Choi and Payne[3] solve the coupled two-state system in the opposite extreme of the adiabatic limit. Their analysis provides, in principle, for calculating beyond the adiabatic limit, by iteration in "orders of adiabaticity." Although their two-state solution is obtained relatively easily, with more than two states the algebra becomes tedious. Their calculation can be extended to accommodate an arbitrary initial superposition of eigenstates of H_0 (done in the Appendix of this paper), and with the conventional norm-of-state definition $P_B(t)=\langle\phi_A(t)\,|\,\phi_A(t)\rangle$ leads to expected ionization and/or decay, plus oscillations between the eigenstates and different decay rates.

Armstrong and Baker have outlined a general procedure for the systematic construction of an appropriate effective Hamiltonian $\hat{H}$ for an ionizing and/or decaying discrete space of any finite dimension[10] (hereinafter referred to as AB). With the appropriate $\hat{H}$ for an ionizing and/or decaying system, "decaying dressed states" are calculated as instantaneous eigenstates of $\hat{H}$. Off-diagonal coupling through virtual continuum transitions[9] is not problematic with this basis of complex-energy states. The continuum contributions are automatically included [to second order in the atom-field interaction $H_{\mathrm{AF}}(t)$] as (real) energy shifts and (imaginary) decay terms. These eigenstates and eigenvalues follow the time evolution of $\hat{H}(t)$, and continuously approach those of free atom-field Hamiltonian H_0 if the interaction is continuously switched off. This theory permits the use of time-independent perturbation theory straightforwardly to calculate dynamical quantities, such as decay rates. The time-profile effects of the atom-field interaction are included through assuming the usual time-dependent Schrödinger equation for the bound-state wave function, with the non-Hermitian effective $\hat{H}$. With the time-dependent, effective Schrödinger equation, it is shown in AB that in the limit of slow variations in the effective atom-field interaction $\hat{H}_{\mathrm{AF}}(t)$, transition amplitudes among the discrete, complex-energy eigenstates are essentially zero. This extends the adiabatic theorem[11] in terms of amplitudes to complex-energy eigenstates. No formal prescription for constructing *modal* occupation *probabilities* is provided for, however, so that the extended adiabatic theorem of AB is a limited one. The eigenstates and their complex energies are to be calculated to first order in the continuum-coupled, *effective* terms in $\hat{H}_{\mathrm{AF}}(t)$, while in near-resonant discrete manifolds, calculations to all orders in the transition matrix elements of $H_{\mathrm{AF}}(t)$ are required. The conventional norm-of-state prescription for total bound-state (nonionization or nondecay) probability $P_B(t)$ is employed in AB [Eq. (16)], which with an initial superposition of eigenstates of H_0 leads to the usual oscillations for $P_B(t)$ and the net ionization rate, even in the adiabatic limit.

The norm-of-state construction for nonionization or nondecay probability $P_B(t)$ has a venerable history.[12] In the earliest applications of this construction, by Weisskopf and Wigner,[12] decay from only a single state was considered, and no differences of consequence result from the alternative construction as argued for in the present paper. In this paper we reconsider the conventional norm-of-state construction of $P_B(t)$ in the context of non-Hermitian dynamics. We find that when the effective Hamiltonian and its eigenstates are considered in the framework of conventional scattering theory the norm-of-state construction for $P_B(t)$ is inconsistent, and in fact erroneous. We provide a consistent construction not only for $P_B(t)$ but also for individual modal occupation probabilities at all intermediate times. We focus for specificity upon the multiphoton ionization problem because the atom-field interaction realistically vanishes in the remote past and future, which permits invocation of the standard considerations from scattering theory, to infer the correct construction of transition amplitudes. One may realistically consider also a semiclassical regime, with arbitrary modulation of decay rates of different modes, leading to an essentially unique construction for intermediate transition amplitudes which is consistent with the infinite-time limit,

where the scattering matrix and adiabatic limit exist in the strict sense.

Also, in analyzing the multiphoton ionization problem we wish to reemphasize the utility of the procedure in AB for obtaining decay rates in a very direct fashion. It would seem necessary, however, that Eq. (16) for $P_B(t)$, a norm-of-state construction, and subsequent developments in AB should be modified in accordance with the analysis and conclusions set forth in this paper.

Although we explicitly consider here the non-Hermitian dynamics of multiphoton ionization, our analysis is performed in a sufficiently general framework that our conclusions apply to any ionizing or decaying discrete space, such as the decay of K_0 mesons to the pion continuum. Whenever phase-shifting processes such as atomic collisions or spontaneous photon emission become important effects, an appropriate density-matrix extension of the present results is easily constructed.

Transition and occupation probabilities defined for an effective non-Hermitian system must take into account the lack of unitarity in the decaying subspace in an overall consistent fashion. Consider an atom-plus-field system with free Hamiltonian $H_0=H_A+H_F$. The field impinges upon the atom, rising to full strength in the atomic neighborhood sufficiently slowly that the interaction $H_{\rm AF}(t)$ may be regarded as adiabatically "switched on." We imagine a slowly varying field envelope, or amplitude, and that it is practically monochromatic. Suppose that the atom is initially in a superposition of eigenstates of the atomic Hamiltonian H_A, say $|1(0)\rangle$ and $|2(0)\rangle$. Under the conditions described, this initial state, which we write as $|0\rangle=c_1|1(0)\rangle+c_2|2(0)\rangle$, evolves under the appropriate effective Hamiltonian $\hat{H}$ (acting only in the atomic subspace) into the state[10] (we take $\hbar=1$ throughout this paper)

$$|t\rangle=c_1\exp\left[-i\int_0^t\lambda_1(t')dt'\right]|1(t)\rangle + c_2\exp\left[-i\int_0^t\lambda_2(t')dt'\right]|2(t)\rangle\ , \tag{1}$$

where c_1 and c_2 are unchanged and $|1(t)\rangle$ and $|2(t)\rangle$ are the instantaneous complex-energy eigenstates of $\hat{H}(t)$. The complex quantities $\lambda_1(t)$ and $\lambda_2(t)$ are the associated instantaneous eigenenergies. The occupation probabilities of modes $|1(t)\rangle$ and $|2(t)\rangle$ are

$$P_1(t)=|c_1|^2\exp\left[-\int_0^t\gamma_1(t')dt'\right]\ , \tag{2a}$$

$$P_2(t)=|c_2|^2\exp\left[-\int_0^t\gamma_2(t')dt'\right]\ . \tag{2b}$$

The quantities $-\gamma_i$ equal twice the imaginary parts of λ_i. If these modes decayed completely independently, one would have, for the ionization rate at any time t,

$$-\frac{dP_B(t)}{dt}=\gamma_1(t)P_1(t)+\gamma_2(t)P_2(t)\ . \tag{3}$$

Owing to the generally nonzero overlap $\langle 1(t)|2(t)\rangle$, the time derivative of the norm-of-state $\langle t|t\rangle$ does not lead to the result (3), even in the adiabatic limit [see Eq. (16) in AB]. The extra cross-terms in the conventional construction[12] are usually accepted as a natural "interference" among the eigenmodes of a non-Hermitian Hamiltonian.

Of course, if one calculates to a consistent low order in the Hermitian interaction $H_{\rm AF}$, the above overlap of states is, to the given order, effectively zero, being always of higher order. However, in decaying degenerate manifolds, or with intermediate-state resonances in multiphoton ionization, one must calculate to all orders in the resonant, or degenerate, manifolds.

According to the analysis presented in this paper, the ionization rate expression of Eq. (3) is in fact the correct one, at least in the adiabatic limit. This conclusion, and other more general ones, follow from careful consideration of the eigenstates not only of $\hat{H}$, but also of the adjoint operator $\hat{H}^\dagger$. It is known, as discussed in AB and also by Faisal and Moloney,[13] that these two sets of eigenstates constitute biorthogonal sets, each set spanning the discrete subspace.[14] We find that both of these sets occur naturally in a correct theory, and have distinct significance revealed by considerations in the context of scattering theory. Thus Hermitian quantum dynamics is shown to contain the information necessary for its generalization to non-Hermitian quantum dynamics.

The preparation of an unstable, decaying and/or ionizing system is in a strict sense properly regarded as a scattering experiment.[14,15] In general, the scattering theory employed should incorporate also the translational continuum of the ionizing and/or decaying discrete-space system ("atom"). This is crucial, if one considers a semiclassical atom-field interaction $H_{\rm AF}$, in order that certain of the distributions may be defined. In actual calculations involving only the discrete-space dynamics, however, such translational "scaffolding" may be discarded, with the caveat that energy bookkeeping must be done "by hand" among the various subspaces.

Some of our conclusions have been discussed elsewhere.[16] In this paper we present additional discussion and detail, and in an appendix illustrate our considerations in detail with the general two-state non-Hermitian system.

The plan of this paper is as follows. In Sec. II we define the illustrative dynamical model. For completeness we review the derivation of the effective Hamiltonian $\hat{H}$ for a decaying discrete space. The non-Hermiticity comes about through the irreversible coupling to an energy-conserving continuum.[17,18] In the process we show that the eigenstates of $\hat{H}(t)$ are projections of Lippmann-Schwinger ("dressed") incoming states, satisfying an initial-state boundary condition, onto the discrete reference space of the noninteracting system. Further, we find that the eigenstates of $\hat{H}^\dagger(t)$ are projections of Lippmann-Schwinger (dressed) outgoing states, satisfying a final-state condition, onto the discrete reference space of the noninteracting system. In Sec. III the considerations of Sec. II are repeated for the time-dependent Schrödinger equation. This leads to time-dependent effective Schrödinger equations using both $\hat{H}(t)$ and $\hat{H}^\dagger(t)$, with states in the first case satisfying an initial-state condition and, in the second case, states satisfying a final-state condition. In Sec. IV we employ the S-matrix aspects of the states evolved under $\hat{H}$ and $\hat{H}^\dagger$, as established in Sec. III, to construct transition and occupation amplitudes for in-

dividual complex-energy eigenstates and for the total bound-state probability $P_B(t)$. An interpolating construction is provided to define individual-mode occupation probabilities for intermediate times, consistent with the long-time S-matrix results in the adiabatic limit. These probabilities satisfy the consistency requirement that *independent* decay from each mode, as manifest in the S matrix, requires that each mode decays independently *at all times* at a rate proportional to its instantaneous probability. With our constructions, the total bound-state probability is at all times the sum of individual-state probabilities. These results are obtained in Sec. V, where the adiabatic limit is evaluated in detail. With our construction of *total* nonionization probability $P_B(t)$, oscillations do not occur through nonzero overlap of different eigenstates of $\hat{H}(t)$. Oscillations in time *would* occur for the probability of any coherent superposition state, however, as is to be expected. In Sec. VI we consider the resolvent-operator solutions of the non-Hermitian dynamical problem. This procedure is suitable during periods of constant interaction. We emphasize that the appropriate bases for utilization of the resolvents for $\hat{H}$ and $\hat{H}^\dagger$ are their associated complex-energy (dressed) eigenstates. In the Appendix we illustrate the application of our theory for the general non-Hermitian two-state system. We extend the Payne-Choi adiabatic iterative technique[3] to solve the time-dependent effective Schrödinger equations with arbitrary initial- and final-state conditions. The naturalness of our construction for transition amplitudes, using the biorthogonal states as dictated by S-matrix considerations, is quite apparent in this Schrödinger picture calculation. We also calculate the eigenvalues and eigenstates as direct solutions of the eigenvalue problem, as advocated in AB. The utility of this approach is apparent. Finally, the nature of the nonzero overlap of nondegenerate eigenstates is explicitly exhibited.

II. EFFECTIVE HAMILTONIANS AND EIGENSTATES

Let us define a particular dynamical process, which, in fact, has features of more general problems. Imagine a composite system consisting of an atom (or other ionizable system) plus a localized packet of photons. The packet, of course, will be a superposition of photon momenta of a narrow range of values. Before some "remote" past time t_i, we imagine the packet to be sufficiently far removed from the atom that the atom-field interaction is zero. The packet impinges upon the target atom with possible ionization as a result; that is, an electron perhaps makes a transition from its initial bound state to the ionization-continuum states. Subsequently, the residual photons, and electron (and any other fragments), if ionization occurs, separate into distinct subsystems, completely noninteracting after some remote future time t_f. This description is close to what happens, in fact, in a laboratory laser ionization of atoms and molecules.

We construct an analyzable model of the essential features of this process as follows. The total Hamiltonian H is expressed as

$$H = H_A + H_F + H_{\mathrm{AF}}(t) \ . \tag{4}$$

H_A is the Hamiltonian for the isolated atom with its constant Coulomb field. H_F is the Hamiltonian for the radiation field and $H_{\mathrm{AF}}(t)$ is the atom-field interaction. It is essentially immaterial to our resultant theory whether H_{AF} is a constant quantum field-atom interaction or a time-dependent semiclassical interaction. Appropriate changes can be made at different points of the development, leading to essentially the same eventual results for the effective dynamics within the discrete atomic subspace. For specificity, we shall present the development in quantized-field terms.

We may model the above-described interaction process with the device of a time-dependent "profile" function in H_{AF}, rather than work with a spatially localized packet *per se*. The time evolution of the profile function $\eta(t)$ can be required to follow that of any actual pulse profile. In this approach we may also assume a monochromatic field mode, occupied by a definite number M of photons, say, of frequency ω. The profile function $\eta(t)$ should be nonzero only on the time interval between t_i and t_f. In the adiabatic limit, where the interval $t_f - t_i$ is infinite and $\eta(t)$ varies only infinitesimally slowly, we have the familiar situation equivalent to the collision of broad atomic and photon wave envelopes.[18,19] For simplicity we shall consider only a single direction and polarization for the photons. The interaction is written as $H_{\mathrm{AF}}(t) = \eta(t) V$, where V is time independent, and $\eta(t)$ is time-profiled to model that of the imagined packet. We require $\eta(t < t_i) = \eta(t > t_f) = 0$, before and after the interaction. We let $H_0 = H_A + H_F$, and write for the complete system Hamiltonian the expression

$$H(t) = H_0 + H_{\mathrm{AF}}(t) \ . \tag{5}$$

We refer to H_0 as the noninteracting, or "free," Hamiltonian.

Let us denote the eigenstates of the free atom-field system as $|\, i\,\rangle\,|\, n\,\rangle = |\, i,n\,\rangle$. The discrete, atomic-state index i is such that $H_A\,|\, i\,\rangle = E_i\,|\, i\,\rangle$. The ionization-continuum states may be designated as $|\, k,n\,\rangle$, where k is the electron-plus-ion energy and n is some residual number of the photons of frequency ω. Thus $H_0\,|\, k,n\,\rangle = (k + n\omega)\,|\, k,n\,\rangle$. We assume that the number M of photons is sufficient that ionization is an energy-conserving process; let m be the minimum number of photons required, so that $m < M$. We shall ignore free-electron rescattering, and try to calculate the probability that the atom makes a transition from a given initial state to any of the final ionization states $|\, k,M-m\,\rangle$. We assume the rotating-wave approximation, and assume closure holds in the form

$$\int dk \sum_n |\, k,n\,\rangle\langle k,n\,| + \sum_{i,n} |\, i,n\,\rangle\langle i,n\,| = \sum_n |\, n\,\rangle\langle n\,| \left[\int dk\, |\, k\,\rangle\langle k\,| + \sum_i |\, i\,\rangle\langle i\,| \right] = 1 \ . \tag{6}$$

It is convenient to condense the above notation somewhat. There is no ambiguity if we represent the discrete atom-field eigenstates of H_0, i.e., the states $|\, i,n\,\rangle$, by the

notation $|a_r\rangle$. We assume that at most a finite number of the eigenstates of H_A need to be considered explicitly in the analysis. The ionization-continuum states $|k,n\rangle$ we shall represent simply by $|e\rangle$, so that $H_0|e\rangle=e|e\rangle$. Note that $e\geq 0$. We have hereby constructed a reference system of discrete states $|a_r\rangle$ satisfying $H_0|a_r\rangle=\epsilon_r|a_r\rangle$, with $\epsilon_r>0$. Therefore, for times t, $t_i\leq t\leq t_f$, $\eta(t)>0$ and we have a decaying discrete space.[14,17] Unlike the ordinary decay of an excited atomic state, however, the present system decays only during the interval $t_i\leq t\leq t_f$. We shall imagine the state of the composite system to be specified for $t<t_i$ as

$$|i\rangle=\sum_r c_r|a_r\rangle\ . \tag{7}$$

We wish to obtain now an effective Hamiltonian $\hat{H}$ which acts only in the discrete space, but which accounts for the ionization-decay loss of probability from this space. We define the projection operator for this space,

$$P=\sum_r |a_r\rangle\langle a_r|\ . \tag{8}$$

The ionization-continuum projection operator we denote as Q, and it is defined as

$$Q=\int de\,|e\rangle\langle e|\ . \tag{9}$$

Of course, $P^2=P$, $Q^2=Q$, and $QP=PQ=0$, and because of closure as indicated in (6), $P+Q=1$. The essential assumption is that the interacting atom-photon system is effectively an open system, well approximated by the finite, discrete reference space, which overlaps an energy-conserving continuum, suffering thereby irreversible loss of probability. There are, in fact, other continuum modes to which this discrete system is coupled, for example, those corresponding to Rayleigh and Raman processes. We assume that ionization dominates the loss from the discrete reference space. In principle, in any case, these other nonionization processes could be included as part of the reference space.

The exact, dressed eigenstates of $H(t)$ at any reference time t, $t_f\geq t\geq t_i$, satisfy the eigenvalue equation

$$H(t)|\epsilon(t)\rangle=\epsilon|\epsilon(t)\rangle\ . \tag{10}$$

The state $|\epsilon(t)\rangle$ may be obtained in the limit $\beta\rightarrow 0^+$ from either of the states $|\epsilon_\pm(t)\rangle$ defined by

$$[H(t)\mp i\beta]|\epsilon(t)\rangle=\epsilon|\epsilon_\pm(t)\rangle\ . \tag{11}$$

This equation, of course, is simply a rewriting of the Lippmann-Schwinger equation,[19] for any fixed reference value of t:

$$|\epsilon_{r\pm}(t)\rangle=|a_r\rangle+\frac{1}{\epsilon_r-H_0\pm i\beta}H_{\mathrm{AF}}(t)|\epsilon_{r\pm}(t)\rangle\ . \tag{12}$$

The energy ϵ_r in (12), of course, must be the total energy of the system, including translational energy of the atom. It will be conserved overall in these photon-atom scattering solutions, although the discrete-space subenergies will generally be t-dependent quantities. We shall not consider explicitly the atomic-translational states that, along with the photon continuum, give meaning to the expression (12). It must be kept in mind, however, that the atomic-translational continuum must, in principle, be included, particularly if H_{AF} is a semiclassical interaction, in order to give meaning to (12). Note that the operators in (10)—(12) are in the Schrödinger picture, although the states in (12) are interaction-picture states.

By writing the Lippman-Schwinger equivalent of (11), we are able to put the $\pm i\beta$ terms into perspective in the context of scattering theory.[18,19] By including the atomic translational continuum so that ϵ_r is overall a conserved quantity one may form continuous superpositions of the eigenstates $|\epsilon_{r\pm}\rangle$ with energies centered around ϵ_r. This superposition may involve different photon energies and different atomic-translational energies. A superposition of $|\epsilon_{r+}\rangle$ states becomes at remote times $t<t_i$ the corresponding superposition of the states $|a_r\rangle$. Likewise, such superpositions of the $|\epsilon_{r-}\rangle$ states evolve into the corresponding superpositions of the states $|a_r\rangle$ at $t>t_f$, in the remote future.[19] These are the collision packets mentioned earlier. By including the atomic-translational continuum, such a description is possible even with the semiclassical atom-field interaction.

In view of the possibility of constructing collision packets as just described, the states $|\epsilon_{r+}\rangle$ are called "incoming" states, and the states $|\epsilon_{r-}\rangle$ are called "outgoing" states.[19] We shall not require these packets in any direct way, however, and shall continue to refer explicitly to only the discrete indices of the reference P space. The state $|a_r\rangle$ in (11) is simply the discrete-space factor-state coefficient of the overall state.

With the foregoing points in mind we proceed as follows. Working only within the discrete reference space, with the Hamiltonian $H=H_0+H_{\mathrm{AF}}$ for this subspace, we define the discrete-space incoming state $|I(t)\rangle$ and discrete-space outgoing states $|F(t)\rangle$:

$$[H(t)-i\beta]|I(t)\rangle=\epsilon_+(t)|I(t)\rangle\ , \tag{13}$$

and

$$[H(t)+i\beta]|F(t)\rangle=\epsilon_-(t)|F(t)\rangle\ . \tag{14}$$

Because of the interaction $H_{\mathrm{AF}}(t)$, $|I(t)\rangle$ and $|F(t)\rangle$ acquire ionization-continuum components. The subspace energies $\epsilon_\pm(t)$ will be time dependent, and will have small imaginary components which vanish as $\beta\rightarrow 0$, for the exact states $|I\rangle$ and $|F\rangle$. We now eliminate from direct consideration the ionization-continuum components of $|I\rangle$ and $|F\rangle$ in an approximation which will leave the approximate energies $\epsilon_\pm$ to be complex (conjugate) energies.

Apply the projection operators P and Q to (13) and obtain the following set of equations:

$$H_{0qq}|I_q\rangle+H_{\mathrm{AF}qp}|I_p\rangle-i\beta|I_q\rangle=\epsilon_+|I_q\rangle\ , \tag{15}$$

and

$$H_{0pp}|I_p\rangle+H_{\mathrm{AF}pq}|I_q\rangle+H_{\mathrm{AF}pp}|I_p\rangle-i\beta|I_p\rangle=\epsilon_+|I_p\rangle \tag{16}$$

leaving t as an implicit parameter. We have defined $H_{0qp}=QH_0P$, etc. A sum over the corresponding space is implied with repeated indices. We shall neglect rescatter-

ing of the ionization components by setting $H_{\mathrm{AF}qq}=0$.

A similar set of equations is obtained from (14). Solving both sets for their $\mathcal{Q}$-space components and eliminating these in favor of the $\mathcal{P}$-space components leads finally to the expressions

$$\left[H_{0pp}+H_{\mathrm{AF}pp}+H_{\mathrm{AF}pq}\frac{1}{\epsilon_+-H_{0qq}+i\beta}H_{\mathrm{AF}qp}-i\beta\right]|I_p\rangle=\epsilon_+|I_p\rangle\ , \tag{17a}$$

and

$$\left[H_{0pp}+H_{\mathrm{AF}pp}+H_{\mathrm{AF}pq}\frac{1}{\epsilon_--H_{0qq}-i\beta}H_{\mathrm{AF}ap}+i\beta\right]|F_p\rangle=\epsilon_-|F_p\rangle\ . \tag{17b}$$

With the definitions

$$\tilde{H}_{\mathrm{AF}}+H_{\mathrm{AF}pp}+H_{\mathrm{AF}pq}\frac{1}{\epsilon_+-H_{0qq}+i\beta}H_{\mathrm{AF}qp} \tag{18}$$

and

$$\hat{H}=H_{0pp}+\tilde{H}_{\mathrm{AF}}\ , \tag{19}$$

we may write Eqs. (17) in the form

$$[\hat{H}(t)-i\beta]P\,|I(t)\rangle=\epsilon_+(t)P\,|I(t)\rangle\ , \tag{20}$$

and

$$[\hat{H}^\dagger+i\beta]P\,|F(t)\rangle=\epsilon_-(t)P\,|F(t)\rangle\ . \tag{21}$$

We now permit $\beta\to 0^+$, and evaluate (20) and (21) to second order in H_{AF}. This requires that ϵ_+ in the denominator of (18) be replaced by the zeroth-order energy appropriate to the states $P\,|I\rangle$ and $P\,|F\rangle$ being calculated, that is, the appropriate ϵ_r. Defining $P\,|I\rangle=|\phi\rangle$ for the eigenstate of $\hat{H}$ and $P\,|F\rangle=|\bar{\phi}\rangle$ for the eigenstates of $\hat{H}^\dagger$, and denoting the complex-valued energies by λ, the results take the form

$$\hat{H}(t)\,|\phi(t)\rangle=\lambda(t)\,|\phi(t)\rangle\ , \tag{22}$$

and

$$\hat{H}^\dagger(t)\,|\bar{\phi}(t)\rangle=\lambda^*(t)\,|\bar{\phi}(t)\rangle\ , \tag{23}$$

where the asterisk denotes ordinary complex conjugation.

To second order, the effective interaction on the discrete space may be written as

$$\hat{H}_{\mathrm{AF}}(t)=H_{\mathrm{AF}pp}(t)S(t)-i\Gamma(t)\ . \tag{24}$$

The "shift" operator $S(t)$ may be expressed in the convenient general form

$$S(t)=PH_{\mathrm{AF}}(t)\,\text{⨍}\,de\,|e\rangle\langle e\,|H_{\mathrm{AF}}(t)\frac{1}{PH_0P-e}P\ , \tag{25}$$

with respect to the basis states $|a_r\rangle$. The symbol ⨍ denotes a principal-value integration. The decay operator $\Gamma(t)$ is responsible for attenuation of $\mathcal{P}$-space probabilities. It may be conveniently expressed in the form

$$\Gamma(t)=\pi H_{\mathrm{AF}}(t)\int de\,|e\rangle\langle e\,|H_{\mathrm{AF}}(t)\delta(PH_0P-e)P \tag{26}$$

valid to second order in $H_{\mathrm{AF}}(t)$, with respect to the basis states $|a_r\rangle$. The effective interaction defined by (24)—(26) will be used in (22) and (23), with $\hat{H}$ given in (19), to define our bases of decaying dressed states, the $|\phi\rangle$'s and the $|\bar{\phi}\rangle$'s.

From the above considerations we see that the eigenstates $|\phi\rangle$ of $\hat{H}(t)$ are the $\mathcal{P}$-space projections of the incoming eigenstates of $H(t)$. The eigenstates of $\hat{H}^\dagger$ are the $\mathcal{P}$-space projections of outgoing eigenstates of $H(t)$. These results lead to important consequences for the construction of transition amplitudes. These consequences will be brought out in Sec. IV.

A further aspect of the eigenstates $\hat{H}$ and $\hat{H}^\dagger$ should be noted. In terms of perturbation theory, the Lippmann-Schwinger representation shows that the exact incoming and outgoing states approach a unique eigenstate of H_0 as the interaction $H_{\mathrm{AF}}(t)$ vanishes. This is expected to be true also for the complex-energy eigenstates,[14] barring degeneracy. Furthermore, to the extent that an adiabatic theorem is valid for the complex-energy eigenstates, we expect that the association between them and the eigenstates of H_0 will also be a dynamic one. As will be shown in Sec. IV, the state $|a_r\rangle$ evolves adiabatically under $\hat{H}$ into the corresponding eigenstate $|\phi_r(t)\rangle$, while the eigenstate $|\bar{\phi}_r(t)\rangle$ evolves adiabatically under $\hat{H}^\dagger$ toward the state $|a_r\rangle$. That is, the states $|\phi_r\rangle$ will be required to satisfy an initial-state condition, whereas the states $|\bar{\phi}_r\rangle$ will be required to satisfy a final-state condition.

The states $|\phi_r(t)\rangle$ and $|\bar{\phi}_s(t)\rangle$ also satisfy a biorthogonality relation for all t.[14] This is easily established. Because of the eigenvalue equation (23), we also have

$$\langle\bar{\phi}_s(t)\,|\hat{H}(t)=\lambda_s(t)\langle\bar{\phi}_s(t)\,|\ . \tag{27}$$

That is, the states $|\bar{\phi}_s\rangle$ are left eigenstates of $\hat{H}$. Therefore, using (22), we find

$$\langle\bar{\phi}_s(t)\,|\hat{H}(t)\,|\phi_r(t)\rangle=\lambda_s\langle\bar{\phi}_s\,|\phi_r\rangle=\lambda_r\langle\bar{\phi}_s\,|\phi_r\rangle\ . \tag{28}$$

Barring degeneracy, therefore,

$$\langle\bar{\phi}_s(t)\,|\phi_r(t)\rangle=0 \tag{29}$$

for $r\neq s$, for all times t. At any value of t we may impose a normalization such that in (29), for $r=s$, we obtain the value 1. We shall denote states which have been normalized in this way as $|A_r(t)\rangle$ and $|\bar{A}_r(t)\rangle$. This defines biorthonormal sets $\{|A_r\rangle\}$ and $\{|\bar{A}_s\rangle\}$ satisfying the equations

$$\hat{H}(t)\,|A_r(t)\rangle=\lambda_r(t)\,|A_r(t)\rangle\ , \tag{30}$$

$$\hat{H}^\dagger(t)\,|\bar{A}_r(t)\rangle=\langle\lambda_r^*(t)\,|\bar{A}_r(t)\rangle\ , \tag{31}$$

and

$$\langle\bar{A}_s(t)\,|A_r(t)\rangle=\delta_{r,s}\ . \tag{32}$$

In general, the states $|\phi_r(t)\rangle$ and $|\bar{\phi}_r(t)\rangle$ which evolve dynamically under $\hat{H}$ and $\hat{H}^\dagger$, respectively (as will be demonstrated in Sec. III), will have amplitude coefficients (in terms of expansions with the states $|A_r\rangle$ and $|\bar{A}_r\rangle$) with modulus less than the value 1, due to the ionization and/or decay. This point will be illustrated in some detail in Sec. V, where we consider the adiabatic limit in general. We shall refer to the states $|\phi\rangle$ and $|\bar{\phi}\rangle$ as dynamic states, and the reference bases $|A\rangle$ and $|\bar{A}\rangle$ as "kinematic" states.

Finally, we note that in terms of the biorthonormal kinematic states, closure takes the form[14]

$$\sum_{r\in\mathscr{P}} |A_r(t)\rangle\langle\bar{A}_r(t)| = \sum_{r\in\mathscr{P}} |\bar{A}_r(t)\rangle\langle A_r(t)| = I \ . \tag{33}$$

III. THE TIME-DEPENDENT SCHRÖDINGER EQUATIONS

We consider now the derivation of an effective time-dependent Schrödinger equation for the $\mathscr{P}$-space amplitudes. It is, of course, the time-dependent equation that describes the transition dynamics in the evolution of the states of the system.

We take as a starting point the exact Schrödinger equation

$$H(t)|\psi(t)\rangle = i\frac{d}{dt}|\psi(t)\rangle \ . \tag{34}$$

The operator $H(t)$ is assumed to be as described in Eq. (5), which incorporates an interaction profile function $\eta(t)$, describing the interaction between the radiation field and the discrete ionizing system atom. With the operators P and Q as specified in Eqs. (8) and (9), we form two equations from (34):

$$P[H_0+H_{\rm AF}(t)](P+Q)|\underline{\psi}(t)\rangle = i\frac{d}{dt}P|\psi(t)\rangle \ , \tag{35}$$

$$Q[H_0+H_{\rm AF}(t)](P+Q)|\psi(t)\rangle = i\frac{d}{dt}Q|\psi(t)\rangle \ . \tag{36}$$

Defining $|\psi_q\rangle = Q|\psi\rangle$, $H_{{\rm AF}pq}=PH_{\rm AF}Q$, etc., as before, and again neglecting $QH_{\rm AF}Q$ we obtain from (36)

$$i\frac{d}{dt}|\psi_q\rangle = H_{0qq}|\psi_q\rangle + H_{{\rm AF}qp}|\psi_p\rangle \ , \tag{37}$$

which leads to

$$\frac{d}{dt}(e^{iH_{0qq}t}|\psi_q\rangle) = -ie^{iH_{0qq}t}H_{{\rm AF}qp}|\psi_p\rangle \ . \tag{38}$$

We shall assume the atom is prepared so that, at time t_i, it is in some $\mathscr{P}$-space state. Therefore, we integrate (38) subject to the (otherwise arbitrary) initial condition $Q|\psi(t_i)\rangle = 0$, to obtain

$$|\psi_q(t)\rangle = -ie^{-iH_{0qq}t} \times \int_{t_i}^{t} e^{iH_{0qq}t'}H_{{\rm AF}qp}(t')|\psi_p(t')\rangle dt' \ . \tag{39}$$

Substituting this result back into (35) yields

$$(H_{0pp}+H_{{\rm AF}pp})|\psi_P(t)\rangle - iH_{{\rm AF}pq}(t)e^{-iH_{0qq}t}\int_{t_i}^{t} e^{iH_{0qq}t'}H_{{\rm AF}qp}(t')|\psi_P(t')\rangle dt' = i\frac{d}{dt}|\psi_P(t)\rangle \ . \tag{40}$$

To zeroth order in $H_{\rm AF}$,

$$|\psi_p(t')\rangle = e^{-iH_{0pp}(t'-t_i)}|\psi_p(t_i)\rangle \ . \tag{41}$$

Defining

$$\Sigma = \int_{t_i}^{t} dt' e^{iH_{0qq}t_i}\eta(t')V_{qp}e^{-iH_{0pp}(t'-t_i)}|\psi_p(t_i)\rangle \tag{42}$$

we may write

$$\Sigma = \int_{t_i}^{t_f} dt'\Theta(t-t')e^{iH_{0qq}t'}\eta(t')V_{qp} \times e^{-iH_{0pp}(t'-t_i)}|\psi_p(t_i)\rangle \ , \tag{43}$$

where $\Theta(t-t')$ is the Heaviside function satisfying

$$\Theta(t-t') = \begin{cases} 0, & t<t' \quad (44a) \\ 1, & t\geq t' \ . \quad (44b) \end{cases}$$

Using the expression (9) for Q, and the fact that $H_0|e\rangle\langle e| = e|e\rangle\langle e|$, we now find

$$\Sigma(t) = \int de \int_{t_i}^{t_f} dt' e^{iet'}|e\rangle\langle e|VPe^{-iH_{0pp}(t'-t_i)} \times \Theta(t-t')\eta(t')|\psi_p(t_i)\rangle \ . \tag{45}$$

Let us write $\eta(t')$ in terms of its Fourier transform $\tilde{\eta}(k)$:

$$\eta(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\eta}(k)e^{ikt}dk \ . \tag{46}$$

In the adiabatic limit, where $d\eta/dt \approx 0$, $\tilde{\eta}(k) = 2\pi\delta(k)$. Also, recall that

$$\Theta(t-t') = \lim_{\beta\to 0^+}\left[\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{iz(t-t')}}{z-i\beta}dz\right] . \tag{47}$$

Performing the integrations over z and t', we find from (45)–(47)

$$\Sigma(t) = \frac{1}{2\pi i}\int de \int dk\, |e\rangle\left\langle e\left|\frac{V\tilde{\eta}(k)e^{i(k+e-H_{0pp})t}}{k+e-H_{0pp}-i\beta}e^{iH_{0pp}t_i}\right|\psi_p(t_i)\right\rangle . \tag{48}$$

We have anticipated in this result that eventually $t_i\to-\infty$ and $t_f\to+\infty$ in doing the t' integration.

To proceed further, it is necessary to make assumptions regarding the profile function $\eta(t)$, or equivalently, its

transform $\tilde{\eta}(k)$. We shall assume adiabatic variation, which with the delta function in the k integration in (48) gives the result

$$\Sigma(t)=-ie^{iH_{0qq}t}\int de\,|\,e\rangle\left\langle e\left|H_{\mathrm{AF}}(t)\frac{1}{e-H_{0pp}-i\beta}\right|\psi_p(t)\right\rangle . \tag{49}$$

This expression substituted into Eq. (40) yields finally the sought-after result:

$$[H_{0pp}+H_{\mathrm{AF}pp}(t)]\,|\,\psi_p(t)\rangle+H_{\mathrm{AF}pq}(t)\int de\,|\,e\rangle\left\langle e\left|H_{\mathrm{AF}}\frac{1}{H_{0pp}-e+i\beta}\right|\psi_p(t)\right\rangle=i\frac{d}{dt}\,|\,\psi_p(t)\rangle . \tag{50}$$

It is observed that this expression is simply equivalent to

$$\hat{H}(t)\,|\,\psi_p(t)\rangle=i\frac{d}{dt}\,|\,\psi_p(t)\rangle , \tag{51}$$

where $\hat{H}$ is

$$\hat{H}(t)=H_{0pp}+\tilde{H}_{\mathrm{AF}}(t) , \tag{52}$$

the same as defined earlier; $\tilde{H}_{\mathrm{AF}}$ is defined in Eqs. (24)—(26), valid to second order in H_{AF}. Equation (51) is the effective time-dependent Schrödinger equation for the evolution of the $\mathscr{P}$-space states.

We observe from (48) that the effective Hamiltonian $\hat{H}(t)$ is in general not independent of the details of the profile function $\eta(t)$. Because the matrix elements $\langle e\,|\,V\,|\,\psi_p\rangle$ are usually slowly varying functions of e, the requirement of adiabatic variation should not, however, be a serious restriction. The additional frequency dependence in the dynamics will be largely absorbed in the expansion coefficients in the wave function, as determined by the time-dependent Schrödinger equation. The time-dependent perturbation theory has been discussed in AB.

A more serious approximation is that in (41), which neglects perturbative influence on the P-state wave function. It should not, however, usually result in dramatic changes in the dynamics, at least from recombination, unless the decay products are somehow confined.[20]

It remains to obtain the effective time-dependent Schrödinger equation for $\mathscr{P}$-space states satisfying an outgoing, or final-state condition, as described for the eigenstates of $\hat{H}^{\dagger}$ in Sec. II. These will be required in the construction of transition amplitudes, as performed in Sec. IV, utilizing also their property as scattering states.

The desired equation is readily obtained by repeating the analysis similar to that leading to (51). The important and essential difference is that instead of requiring $|\,\psi_q(t_i)\rangle=0$, we require a final $\mathscr{P}$-space state with $|\,\psi_q(t_f)\rangle=0$. The appropriate Heaviside function in the extended-time integration, corresponding to that in (45), is $\Theta(t'-t)$. In the Fourier transform representation of this function the pole occurs in the lower-half z plane, so that instead of $-i\beta$ in (47) we have $+i\beta$ in the denominator. The rest of the analysis proceeds parallel to the previous, leading finally, again in the adiabatic limit, to the result

$$\hat{H}^{\dagger}(t)\,|\,\bar{\psi}_p(t)\rangle=i\frac{d}{dt}\,|\,\bar{\psi}_p(t)\rangle , \tag{53}$$

where here $\hat{H}^{\dagger}$ is the Hermitian conjugate of (52). The bar on $|\,\psi_p\rangle$ is to designate that the state which solves (53) is required to satisfy a final-state condition, and at remote future time t_f becomes identical to some state for which one wishes to determine the amplitude for a transition. Again, the adiabatic limit is not a serious limitation. As described for the states satisfying (51), with an incoming condition, the state may be expressed as a linear combination of instantaneous eigenstates of $\hat{H}^{\dagger}$, and the coefficients may be determined at different times by the use of (53) with time-dependent perturbation theory.[10]

In terms of the notation of Sec. II we summarize our results thus far for the time-dependent Schrödinger equations:

$$\hat{H}(t)\,|\,\phi_i(t)\rangle=i\frac{d}{dt}\,|\,\phi_i(t)\rangle , \tag{54}$$

$$\hat{H}^{\dagger}(t)\,|\,\bar{\phi}_f(t)\rangle=i\frac{d}{dt}\,|\,\bar{\phi}_f(t)\rangle . \tag{55}$$

Furthermore, the dynamical equations (54) and (55) must be supplemented by subsidiary initial- and final-state conditions:

$$\lim_{t\to t_i}\,|\,\phi_i(t)\rangle=|\,i\rangle , \tag{56}$$

$$\lim_{t\to t_f}\,|\,\bar{\phi}_f(t)\rangle=|\,f\rangle . \tag{57}$$

The states $|\,i\rangle$ and $|\,f\rangle$ are permitted to be any states in $\mathscr{P}$ space, which may be expressed as linear combinations of the eigenstates $|\,a_r\rangle$ of H_0. This assumes that the initial and final reference times t_i and t_f are such that the interaction H_{AF} is zero.

An important additional point should be noted. If one solves the dynamical equations (54) and (55) and wishes to impose initial- and final-state conditions at times t_0 and t_1, where $t_f\geq t_1>t_0\geq t_i$, one requires in this case

$$\lim_{t\to t_0}\,|\,\phi_i(t)\rangle=|\,\phi_0(t_0)\rangle , \tag{56'}$$

$$\lim_{t\to t_1}\,|\,\bar{\phi}_1(t)\rangle=|\,\bar{\phi}_1(t_1)\rangle . \tag{57'}$$

The states $|\,\phi(t_0)\rangle$ and $|\,\bar{\phi}_1(t_1)\rangle$ here must themselves be solutions of (54) and (55), and be expressible as linear combinations of the bases $|\,A_r(t_0)\rangle$ and $|\,\bar{A}_r(t_1)\rangle$, defined by Eqs. (30)—(32). The choice of normalization on the coefficients in the linear expansion for the state $|\,\phi_0(t_0)\rangle$ will be dictated by whether the atomic system has been prepared (or "measured") at this time t_0 to be in an un-ionized state. This relates to unitarity. More will be said in this regard, after the constructions for transition amplitudes are provided in Secs. IV and VI.

IV. TRANSITION AMPLITUDES AND BOUND-STATE PROBABILITIES

In order to make predictions with this theory one must specify how to construct transition amplitudes. In conventional quantum mechanics, one forms inner products of states on a basis of eigenstates of Hermitian operators. Such eigenstates have simple orthogonality properties, which fact leads to a simple algorithm. The results have a transparent interpretation in terms of distributions of measurements of observables. In the present case, the biorthogonality requires additional considerations.

Fortunately, we do not have to search far afield to find a resolution of the problem. The clue is found in the observation that the states $|\phi\rangle$ and $|\bar{\phi}\rangle$ are the projections of "in" and "out" states of S-matrix theory. Recall that to construct the amplitude for a given initial state $|i\rangle$ to undergo an interaction, and subsequently make a transition to a specific final state $|f\rangle$, one forms the S-matrix element,[19] in the interaction picture,

$$S_{f,i}=\langle f|S|i\rangle=\langle f(\text{out})|i(\text{in})\rangle \ . \tag{58}$$

The states $|i(\text{in})\rangle$ and $|f(\text{out})\rangle$ are related to the states $|i\rangle$ and $|f\rangle$ by the Lippmann-Schwinger equations as described in Sec. II. In general, there will be energy- and momentum-conserving delta functions in these matrix elements, in association with the continuum-space components of the wave functions. For the transitions within our model discrete space, however, we need only to be concerned with the appropriate subspace inner products, which will not result in these delta functions. As long as we keep in mind the overall energy balance, it is adequate to consider explicitly only these subspace matrix elements, formed in precisely the manner indicated in (58).

Let us consider, then, a given initial state $|i\rangle\in P$, which may be expressed as $|i\rangle=\sum_r c_r|a_r\rangle$. We wish to find the amplitude after the interaction $\tilde{H}_{\text{AF}}(t)$ has run its course, that the system will be in a specific final state $|f\rangle=\sum_s \bar{c}_s|a_r\rangle$. Noting the intrinsic S-matrix nature of the present theory, we set up the following algorithm.

(1) First, determine that particular incoming state $|\phi_i(t)\rangle$ which evolves from the initial state $|i\rangle$, as the interaction becomes nonzero after some reference time t_i. It is generally most convenient, for the discrete-space transitions, to construct these states as solutions of the effective Schrödinger equation (54), subject to the initial-state condition (56).

(2) Second, determine that particular outgoing state $|\bar{\phi}_f(t)\rangle$ which is on a final-state trajectory toward $|f\rangle$. This may be done on the discrete space by solving the effective Schrödinger equation (55), subject to the final-state condition (57).

(3) Third, form the desired transition amplitude on the discrete space as in (58). In terms of the ϕ notation for the $\mathscr{P}$-space projections of exact scattering states we have, therefore, in the Schrödinger picture,

$$S_{f,i}=\langle\phi_f(t)|\phi_i(t)\rangle \ . \tag{59}$$

It should be kept in mind that recombination is ignored in the approximation (58), in a way that is equivalent to ignoring terms such as $\langle f(\text{out})|Q|i(\text{in})\rangle$ in the exact transition amplitude. However, the result (58) contains the continuum-induced energy shifts in the state ϕ, as well as the decay-loss terms, in the Markov approximation. Within these limits, the expression (59) thus provides the amplitude for $\mathscr{P}$-space transitions, corresponding to the atom-field system, being initially in some P-state $|i\rangle$, and ending up finally in a P-state $|f\rangle$ after the photons and atom have ceased to interact. The probability $P_{f\leftarrow i}$ for this particular transition is then simply

$$P_{f\leftarrow i}(t_f)=|S_{f,i}|^2 \ . \tag{59'}$$

The total final probability of finding the system still in $\mathscr{P}$ space, that is, of nonionization of the atom, is found by summing over all possible final bound states. This gives

$$P_B(t_f)=\sum_{f\in\mathscr{P}}|S_{f,i}|^2 \ . \tag{60}$$

As will be seen in later illustrations, the results (59′) and (60) will be independent of the reference-time parameter t in the states used in these constructions.

It is of considerable interest also to find intermediate-time occupation amplitudes for the discrete $\mathscr{P}$-space states. That is, given an initial state $|i\rangle=\sum_r c_r|a_r\rangle$ for $t<t_i$, we wish to determine the amplitude $c_r(t)$ at an intermediate time t, $t_f>t>t_i$, that the system would be measured to be in some specific complex-energy eigenstate (characterized by decay pattern and Stark-shifted energy spectrum). More generally, one could construct intermediate-time amplitudes for the system to be found in a state which *dynamically* evolves into a particular asymptotic (noninteracting) final state $|f\rangle$. This would require actual calculation of $|\bar{\phi}_f(t)\rangle$, using the effective Schrödinger equation (55), subject to the final-state condition (57). In general, however, it is quite adequate and more convenient to use as an intermediate-time reference basis the intermediate-time eigenstates $\{|A_r(t)\rangle\}$ which, modulo the integrated-energy exponential factors, evolve adiabatically from the corresponding states $\{|a_r\rangle\}$ (see Sec. V). A convenient and useful construction is the amplitude to find the system at intermediate times in a selected *superposition state* which adiabatically evolves into the corresponding superposition final state.

Let us express the incoming state $|\phi_i(t)\rangle$ *dynamically* evolved from the initial state $|i\rangle=\sum_r c_r|a_r\rangle$, according to the Schrödinger equation (54) (subject to 56), as

$$|\phi_i(t)\rangle\sum_r c_r(t)|A_r(t)\rangle \ . \tag{61}$$

With the use of (32) the time-dependent coefficients are given as

$$c_r(t)=\langle\bar{A}_r(t)|\phi_i(t)\rangle \ . \tag{62}$$

The occupation probability at time t for the state $|\phi_i(t)\rangle$ to be found in the state which adiabatically evolves into $|a_r\rangle$ in the remote future is, therefore,

$$P_r(t)=|\langle\bar{A}_r(t)|\phi_i(t)\rangle|^2=|c_r(t)|^2 \ . \tag{63}$$

The expression is readily understandable in the context of S-matrix theory. It is merely the inner product of the

(projected) outgoing Lippmann-Schwinger (dressed) state at time t with the (Schrödinger picture) incoming state. In the limit in which $t \to t_f$, the result (59′) is reproduced, for the particular case $|f\rangle = |a_r\rangle$.

To obtain the intermediate-time occupation probability for the state adiabatically associated with the arbitrary final superposition state $|f\rangle = \sum_r \bar{c}_r |a_r\rangle$ (with $\sum_r |\bar{c}_r|^2 = 1$), we form the inner product of $|\phi_i(t)\rangle$ with the corresponding linear combination of outgoing (projected) Lippmann-Schwinger states, and take the square of the absolute value:

$$P_f(t) = \left| \sum_r \bar{c}_r^* \langle \bar{A}_r(t) | \phi_i(t) \rangle \right|^2 . \tag{64}$$

In general, $P_f(t)$ will exhibit oscillations in time, and the limit $t \to t_f \to \infty$ will not be well defined. This is a well-known phenomenon in superposition-state probabilities in the Schrödinger picture.

The total, intermediate-time bound-state (nonionization or nondecay) probability $P_B(t)$ is given as a sum over any complete set of outgoing states. With the convenient adiabatic basis we thus obtain

$$P_B(t) = \sum_{r \in \mathscr{P}} |\langle \bar{A}_r(t) | \phi_i(t) \rangle|^2 = \sum_{r \in P} |c_r(t)|^2 . \tag{65}$$

In general, this expression will not exhibit the oscillations in t which occur in the norm-of-state construction due to nonorthogonality of eigenstates of $\hat{H}(t)$. In the limit $t \to t_f$, (65) becomes equivalent to (60). In general, the coefficients in (65) will satisfy $\sum_r |c_r(t)|^2 < 1$, because of ionization or decay.

V. THE ADIABATIC LIMIT IN GENERAL

The adiabatic limit is a practical, often realized laboratory situation and is in general a convenient theoretical frame of reference. In this section we shall consider this limit in the context of non-Hermitian dynamics and the complex-energy eigenstates.

We assume that the kinematic problem of finding instantaneous eigenstates $|A_r(t)\rangle$ and $|\bar{A}_r(t)\rangle$ satisfying the orthonormality and closure conditions (30)—(33) has been solved. We consider an arbitrary initial state $|i\rangle \in P$, which evolves according to the dynamical, time-dependent effective Schrödinger equation (54) into the state $|\phi_i(t)\rangle$. We shall assume that $|i\rangle$ has been specified in terms of the eigenstates $|a_r\rangle$ of H_0, as $|i\rangle = \sum_r c_r(t_i)|a_r\rangle$, and seek to determine the expansion coefficients of the state $|\phi_i(t)\rangle$. We express $|\phi_i(t)\rangle$ as

$$|\phi_i(t)\rangle = \sum_s c_s(t) \exp\left[-i \int_{t_i}^t \lambda_s(t')dt'\right] |A_s(t)\rangle , \tag{66}$$

where the λ's are the complex-energy eigenvalues of $\hat{H}(t)$, as defined in (30).

We employ the expansion (66) in the Schrödinger equation (54) to obtain the dynamical equations

$$\sum_s \dot{c}_s(t) \exp\left[-i \int_{t_i}^t \lambda_s(t')dt'\right] |A_s(t)\rangle + \sum_s c_s(t) \exp\left[-i \int_{t_i}^t \lambda_s(t')dt'\right] |\dot{A}_s(t)\rangle = 0 , \tag{67}$$

where the overdot denotes differentiation with respect to time. Using the orthonormality of the $|A_s(t)\rangle$ states expressed in (32), we obtain

$$\dot{c}_r(t) = -\sum_s c_s(t) \exp\left[-i \int_{t_i}^t [\lambda_s(t') - \lambda_r(t')]dt'\right] \times \langle \bar{A}_r(t) | \dot{A}_s(t) \rangle . \tag{68}$$

The outgoing states $|\bar{\phi}_f(t)\rangle$ may be expressed as

$$|\bar{\phi}_f(t)\rangle = \sum_s \bar{c}_s(t) \exp\left[-i \int_{t_f}^t \lambda_s^*(t')dt'\right] |\bar{A}_s(t)\rangle . \tag{69}$$

The time limits in the above exponential integrations have been chosen with regard to the conditions expressed in (56) and (57). With the expansion (69) employed in the appropriate Schrödinger equation (55) we obtain

$$\dot{\bar{c}}_r(t) = -\sum_s \bar{c}_s(t) \exp\left[-i \int_{t_f}^t [\lambda_s^*(t') - \lambda_r^*(t')]dt'\right] \times \langle A_r(t) | \dot{\bar{A}}_s(t) \rangle . \tag{70}$$

Further analysis is simplified somewhat by a rephasing of the amplitudes $c_r(t)$ and $\bar{c}_r(t)$. We define new amplitudes

$$c_r'(t) = e^{-i\sigma_r(t)} c_r(t) \tag{71}$$

and

$$\bar{c}_r'(t) = e^{-i\bar{\sigma}_r(t)} \bar{c}_r(t) , \tag{72}$$

and require that the terms with $r = s$ vanish in Eqs. (68) and (70). This results in the equations

$$i\dot{\sigma}_r(t) + \langle \bar{A}_r(t) | \dot{A}_r(t) \rangle = 0 , \tag{73}$$

$$i\dot{\bar{\sigma}}_r(t) + \langle A_r(t) | \dot{\bar{A}}_r(t) \rangle = 0 . \tag{74}$$

We choose solutions with regard to the initial- and final-state conditions (56) and (57):

$$i\sigma_r(t) = -\int_{t_i}^t \langle \bar{A}_r(t') | \dot{A}_r(t') \rangle dt' , \tag{75}$$

$$i\bar{\sigma}_r(t) = -\int_{t_f}^t \langle A_r(t') | \dot{\bar{A}}_r(t') \rangle dt' . \tag{76}$$

The quantities $|\dot{A}_r(t)\rangle$ and $|\dot{\bar{A}}_r(t)\rangle$ are nonzero only during the rise time and fall time of the interaction. For t lying between the rise and fall of the interaction, $\sigma_r(t)$ and $\bar{\sigma}_r(t)$ depend only on the rise time and fall time, respectively, and not on t. In the following we shall assume that the phases of the expansion coefficients have been chosen so that the diagonal terms ($r = s$) in (68) and (70) may be neglected.

The inner products that occur in (68) and (70) have use-

ful alternative expressions. Differentiating the eigenvalue equation (30) gives

$$\dot{\tilde{H}}(t)\,|\,A_r(t)\rangle+[H_0+\tilde{H}(t)]\,|\,\dot{A}_r(t)\rangle = \dot{\lambda}_r(t)\,|\,A_r(t)\rangle+\lambda_r(t)\,|\,\dot{A}_r(t)\rangle\ . \quad (77)$$

Forming the inner product with $|\,\bar{A}_s(t)\rangle$ and integrating yields

$$\langle\,\bar{A}_s(t)\,|\,\dot{A}_r(t)\rangle=\frac{\langle\,\bar{A}_s(t)\,|\,\dot{\tilde{H}}(t)\,|\,A_r(t)\rangle}{\lambda_r(t)-\lambda_s(t)}\ . \quad (78)$$

Similarly, differentiating (31), etc., leads to

$$\langle\,A_s(t)\,|\,\dot{\bar{A}}_r(t)\rangle=\frac{\langle\,A_s(t)\,|\,\dot{\tilde{H}}^{\dagger}(t)\,|\,\bar{A}_r(t)}{\lambda_r^*(t)-\lambda_s^*(t)}\ . \quad (79)$$

The expressions (78) and (79) may be employed in (69) and (70), and the terms with $r=s$ may be excluded.

The results (78) and (79) establish the possibility of an adiabatic theorem for complex-energy eigenstates. Providing that $\lambda_r(t)\neq\lambda_s(t)$ for any t, then in the limit $\tilde{H}(t)$ varies very slowly one has

$$\langle\,\bar{A}_s(t)\,|\,\dot{A}_r(t)\rangle=\langle\,A_s(t)\,|\,\dot{\bar{A}}_r(t)\rangle\cong 0\ . \quad (80)$$

With (68) and (70), and (66) and (69), we then have the adiabatic incoming and outgoing $\mathscr{P}$-space states

$$|\,\phi_i(t)\rangle=\sum_s c_s(t_i)\exp\left[-i\int_{t_i}^{t}\lambda_s(t')dt'\right]|\,A_s(t)\rangle \quad (81)$$

and

$$|\,\bar{\phi}_f(t)\rangle=\sum_s \bar{c}_s(t_f)\exp\left[-i\int_{t_f}^{t}\lambda_s^*(t')dt'\right]|\,\bar{A}_s(t)\rangle\ . \quad (82)$$

The initial- and final-state conditions (55) and (56) are incorporated in these solutions. It is also implicit that, in the strict sense of the adiabatic limit, t_i and t_f must define an infinite interval t_f-t_i.

For "not too strong" an interaction the $\lambda_r(t)$ are not expected to be degenerate, providing the original unperturbed eigenvalues ϵ_r are not.[14] Otherwise one has a resonance condition which requires special attention, in the form of choosing an alternative linear combination of basis vectors in the degenerate subspace, so that the expressions (78) and (79) have vanishing numerators. We shall not pursue this technical problem further here.

We shall take the vanishing of the expressions in (78) and (79) to define the adiabatic limit in general, with the implication of constant expansion coefficients $c_r(t_i)$ and $\bar{c}_r(t_f)$ as expressed in (81) and (82). The fact that these adiabatic coefficients are constants implies that the occupation probabilities of the states may also be constant in time. As discussed in the Introduction, such a result is not obtained by requiring that the occupation probability of state $|\,\phi_r(t)\rangle$, for example, be given by the square of the absolute value of the inner product between $|\,\phi_r(t)\rangle$ and $|\,\phi_i(t)\rangle$ because of the overlap of the $|\,A_r\rangle$'s. With the construction (63), using (62), we obtain, on the other hand, with $\lambda_r(t)=\epsilon_r(t)-i\gamma_r(t)/2$, where ϵ_r and γ_r are real quantities,

$$P_r(t)=|\,c_r(t_i)\,|^2\exp\left[-\int_{t_i}^{t}\gamma_r(t')dt'\right]\ . \quad (83)$$

Therefore, although these occupation probabilities are not constant, due to ionization decay, there is no comingling of populations and they attenuate independently at their own rate.

To obtain the transition amplitude to an arbitrary final state $|\,f\rangle=\sum_r \bar{c}_r(t_f)\,|\,a_r\rangle$, in the adiabatic limit, we use (81) and (82) with the construction (59) to obtain

$$S_{f,i}=\sum_{r,s}\bar{c}_r^*(t_f)c_s(t_i)\exp\left[-i\int_{t_i}^{t}\lambda_s(t')dt'+i\int_{t_f}^{t}\lambda_r(t')dt'\right]\times\langle\,\bar{A}_s(t)\,|\,A_r(t)\rangle \quad (84)$$

or

$$S_{f,i}=\sum_s \bar{c}_s^*(t_f)c_s(t_i)\exp\left[-i\int_{t_i}^{t_f}\lambda_s(t')dt'\right]\ . \quad (85)$$

As remarked earlier, the reference time t is irrelevant. In the particular case that $|\,f\rangle=|\,a_n\rangle$, one has for the occupation probability P_n after the interaction, using (60),

$$P_n=|\,c_n(t_i)\,|^2\exp\left[-\int_{t_i}^{t_f}\gamma_n(t')dt'\right]\ . \quad (86)$$

This agrees with (83) for $t\to t_f$.

The total bound-state probability for any intermediate time t is, by (65),

$$P_B(t)=\sum_{r\in\mathscr{P}}|\,\langle\,\bar{A}_r(t)\,|\,\phi_i(t)\rangle\,|^2 \quad (87)$$

$$=\sum_{r\in\mathscr{P}}|\,c_r(t_i)\,|^2\exp\left[-\int_{t_i}^{t}\gamma_r(t')dt'\right] \quad (88)$$

in the adiabatic limit, where the coefficients $c_r(t_i)$ are given in (81). To obtain the rate of loss of this probability, we may proceed formally by differentiating (87), and make use of the result (80) and the Schrödinger equations (54) and (55);

$$\frac{dP_B(t)}{dt}=-i\sum_{r\in\mathscr{P}}\left[\langle\,\bar{A}_r\,|\,\hat{H}\,|\,\phi_i\rangle\langle\,\phi_i\,|\,\bar{A}_r\rangle-\langle\,\bar{A}_r\,|\,\phi_i\rangle\langle\,\phi_i\,|\,\hat{H}^{\dagger}\,|\,\bar{A}_r\rangle\right] \quad (89)$$

$$=2\sum_{r\in\mathscr{P}}|\,c_r(t_i)\,|^2[\mathrm{Im}\lambda_r(t)]\times\exp\left[-\int_{t_i}^{t}\gamma_r(t')dt'\right]\ . \quad (90)$$

This result is precisely what one obtains by differentiating (88).

It is seen from the foregoing that our construction of interpolating probability functions for intermediate times, satisfies a consistency condition; namely, the loss rate from each mode is at all times proportional to the occupation probability of that mode. Further, these constructions result in the total bound-state probability being a simple sum of the independent-mode probabilities (or populations), in contrast to norm-of-state construction. These results seem very reasonable, particularly since the decay history of a single mode, shown in (86), is insensitive to

other mode-occupation amplitudes at any intermediate time.

In the limit $t \to t_f$ in (87), we obtain

$$P_B(t_f) = \sum_{r \in \mathscr{P}} |c_r(t_i)|^2 \exp\left[-\int_{t_i}^{t_f} \gamma_r(t')dt'\right] . \quad (91)$$

This is an agreement with the result of forming the inner product $|\phi(t_f)\rangle$ with the state $|a_r\rangle$ and squaring, because the states $|\bar{A}_r\rangle$ continuously approach[14] the states $|a_r\rangle$ as $t \to t_f$. In any case, the asymptotic result agrees with the norm-of-state construction for $P_B(t_f)$, which is to be expected after the interaction, when the reference bases are eigenstates of H_0. It is also worth noting the close similarity between the result (91) for the adiabatic limit and the result for similar substate transition probabilities, where the substates are angular-momentum states (Ref. 19, p. 347).

We conclude this section by considering briefly the possibility that a measurement is performed at some intermediate time t_0, $t_i < t_0 < t_f$, and it is found that ionization has not occurred. In this case, the appropriate initial condition on the state $|\phi_i(t)\rangle$ is incorporated in the solution to the dynamical Schrödinger equation (54) by writing

$$|\phi_i(t)\rangle = \sum_r c_r(t_0) \exp\left[-i\int_{t_0}^{t} \lambda_r(t')dt'\right] |A_r(t)\rangle , \quad (92)$$

in the adiabatic regime. This solution satisfies the intermediate-time initial-state condition as prescribed in (55′); explicitly, this construction satisfies the condition

$$\lim_{t \to t_0} |\phi_i(t)\rangle = \sum_{r \in \mathscr{P}} c_r(t_0) |A_r(t_0)\rangle , \quad (93)$$

where we must have

$$P_B(t_0) = \sum_{r \in \mathscr{P}} |\langle \bar{A}_r(t_0) | \phi_i(t_0)\rangle|^2 = \sum_r |c_r(t_0)|^2 = 1 . \quad (94)$$

If at some later time t_1 we wish to know the amplitude to find the system in a particular P state $|A_r\rangle$, we must form the inner product

$$\langle \bar{A}_r(t_1) | \phi_i(t_1)\rangle = c_r(t_0) \exp\left[-i\int_{t_0}^{t_1} \lambda_r(t')dt'\right] . \quad (95)$$

The probability, of course, is

$$P_r = |c_r(t_0)|^2 \exp\left[-\int_{t_0}^{t_1} \gamma_r(t')dt'\right] . \quad (96)$$

These considerations are relevant for time periods t between the rise and fall of the interaction, when the states are essentially stationary.

VI. NON-HERMITIAN RESOLVENT THEORY

As has been indicated by Eqs. (56′) and (57′) and as illustrated explicitly for the adiabatic state in (92), one may solve the Schrödinger equations (54) and (55) for intermediate-time initial conditions, without direct reference to the asymptotic regimes $t > t_f$ and $t < t_i$ or to the eigenstates of H_0 at these times. We wish to start this section with further discussion for intermediate-time initial- and final-state conditions, and to go beyond the adiabatic limit for which (92) and (93) are appropriate.

Let us imagine our atom-field system has been prepared by measurement to be in some $\mathscr{P}$-space state $|\phi_0\rangle$ at some initial time t_0, $t_i < t_0 < t_f$, corresponding to a nonionized atom. We imagine a second measurement on the system at some later time t_1, such that $t_i < t_0 < t_1 < t_f$, to determine whether it is still nonionized or more specifically, is in some particular $\mathscr{P}$-space state $|\phi_1\rangle$. In order to account completely for the dynamical course of events between t_0 and t_1, and to construct the associated transition amplitude in accord with the procedure using Eqs. (54)–(58), we must solve (54) and (55) for dynamical states $|\phi_0(t)\rangle$ and $|\phi_1(t)\rangle$ and require

$$\lim_{t \to t_0} |\phi_0(t)\rangle = |\phi_0\rangle \quad (97)$$

and

$$\lim_{t \to t_1} |\phi_1(t)\rangle = |\phi_1\rangle . \quad (98)$$

In the present example it is crucial to note that nonionization states $|\phi_0\rangle$ and $|\phi_1\rangle$ *will not* satisfy

$$\langle \phi_0 | \phi_0\rangle = \langle \bar{\phi}_1 | \bar{\phi}_1\rangle = 1 , \quad (99)$$

unless, of course, the interaction $\tilde{H}_{\mathrm{AF}}$ happens to be zero. In particular, column-matrix states normalized to the value 1 do not correspond to nonionized states at these times. The reason for this is that, within the non-Hermitian dynamical framework, the appropriate measure of total bound-state probability at any intermediate time t is defined by the construction (65). Unitarity in this framework requires a careful matching of $\hat{H}(t)$, in the dynamical equations (54) and (55), with the instantaneous normalization of the reference complex-energy states. The appropriate description for a nonionized state $|\phi_0\rangle$ at time t_0 is

$$\sum_{r \in \mathscr{P}} |\langle \bar{A}_r(t_0) | \phi_0\rangle|^2 = 1 . \quad (100)$$

Similarly, the nonionized state $|\bar{\phi}_1\rangle$ should satisfy

$$\sum_{r \in \mathscr{P}} |\langle A_r(t_1) | \bar{\phi}_1\rangle|^2 = 1 . \quad (101)$$

These constraints are most easily incorporated by expanding $|\phi_0\rangle$ and $|\bar{\phi}_1\rangle$ as

$$|\phi_0\rangle = \sum_{r \in \mathscr{P}} c_r(t_0) |A_r(t_0)\rangle \quad (102)$$

and

$$|\phi_1\rangle = \sum_{r \in \mathscr{P}} \bar{c}_r(t_1) |\bar{A}_r(t_1)\rangle , \quad (103)$$

where, using (100) and (101),

$$\sum_r |c_r(t_0)|^2 = \sum_r |\bar{c}_r(t_1)|^2 = 1 . \quad (104)$$

To answer the original question regarding the presence of a nonionized atom at time t_1, given that it is nonionized at time t_0, we must determine the dynamical solution

to (54) and (55), $|\phi_0(t)\rangle$ and $|\phi_1(t)\rangle$, subject to (102)—(104), and form the amplitude

$$S_{1\leftarrow 0}(t_1,t_0)=\langle\bar{\phi}_1(t)\,|\,\phi_0(t)\rangle\ . \tag{105}$$

The corresponding probability is simply

$$P_{1\leftarrow 0}(t_1,t_0)=|\,S_{1\leftarrow 0}(t_1,t_0)\,|^2\ . \tag{106}$$

In the adiabatic limit, and for a single P state $|\,A_r\rangle$ at t_0, the solution to this problem is easily obtained and reproduces the result (96).

With the foregoing discussion in mind, we now consider the question of resolvent technique for a non-Hermitian dynamical system. We shall assume here that a suitable non-Hermitian Hamiltonian $\hat{H}$ has been obtained with which to compute decay from the model discrete reference space. We explore the use of a resolvent operator for the non-Hermitian Hamiltonian.

In order for a resolvant formalism to be applicable there must exist a time interval during which the interaction is changing insignificantly. We shall thus consider the dynamics on an interval of time t_1-t_0, where $t_f>t_1>t_0>t_i$, during which $\hat{H}(t)$ is essentially constant. Following the above discussion, suitable reference bases are the instantaneous eigenstates $|\,A_r(t)\rangle$ and $|\,\bar{A}_r(t)\rangle$ which correspond to projected, fully dressed states satisfying initial- and final-state conditions $|\,A_r(t_i)\rangle = |\,a_r\rangle = |\,\bar{A}_r(t_f)\rangle$. Because we shall be concerned here with the possibility of ionization strictly within the interval t_1-t_0, the initial- and final-state conditions appropriate to solutions of the dynamical equations (54) and (55) are (97) and (98), subject to the expansions (102) and (103) and constrained by (104).

The resolvent operator G_i for $\hat{H}$, with the Schrödinger equation (54), is defined by the equation

$$(z-\hat{H})\hat{G}_i(z)=1\ . \tag{107}$$

For the Schrödinger equation (55), we have a resolvent $\hat{G}_f$,

$$(z-\hat{H}^{\dagger})\hat{G}_f=1\ . \tag{108}$$

Define the projection operators

$$P_r=|\,A_r(t)\rangle\langle\bar{A}_r(t)\,|\ , \tag{109}$$

and

$$P_r^{\dagger}=|\,\bar{A}_r(t)\rangle\langle A_r(t)\,|\ . \tag{110}$$

Because of the closure properties (33) we easily solve (107) and (108) using (109) and (110):

$$\hat{G}_i(z)=\sum_r\frac{P_r}{z-\lambda_r}\ , \tag{111}$$

and

$$\hat{G}_f(z)=\sum_r\frac{P_r^{\dagger}}{z-\lambda_r^*}\ . \tag{112}$$

We readily obtain the nonunitary time-translation operators by Fourier transformation:[15]

$$T_i(t-t_0)=\frac{1}{2\pi i}\sum_{r\in\mathscr{P}}\int_{i\epsilon+\infty}^{i\epsilon-\infty}dz\frac{e^{-iz(t-t_0)}}{z-\lambda_r}P_r \tag{113}$$

and

$$T_f(t-t_1)=\frac{1}{2\pi i}\sum_{r\in\mathscr{P}}\int_{i\epsilon+\infty}^{i\epsilon-\infty}dz\frac{e^{-iz(t-t_1)}}{z-\lambda_r^*}P_r^{\dagger}\ . \tag{114}$$

The integrand has poles in the lower-half z plane in (113) and in the upper-half z plane in (114). Thus

$$T_i(t-t_0)=\Theta(t-t_0)\sum_{r\in\mathscr{P}}e^{-i\lambda_r(t-t_0)}P_r\ , \tag{115}$$

$$T_f(t-t_1)=\Theta(t_1-t)\sum_{r\in\mathscr{P}}e^{-i\lambda_r^*(t-t_1)}P_r^{\dagger}\ . \tag{116}$$

Notice that the operators T_i and T_f satisfy semigroup properties

$$T_i(t)T_i(t')=T_i(t+t') \tag{117}$$

and

$$T_f(t)T_f(t')=T_f(t+t')\ . \tag{118}$$

Also

$$T_f^{\dagger}(t-t_1)T_i(t-t_0)=T_i(t_1-t_0) \tag{119}$$

and

$$T_i^{\dagger}(t_i-t_0)T_f(t-t_1)=T_f(t_0-t_1)\ . \tag{120}$$

One should note that during a time period of constant $\hat{H}$, transitions from one complex-energy state in $\mathscr{P}$ space to another do not occur, and are not expected, by the adiabatic theorem. Ionization decay, of course, will continue independently from each complex-energy eigenstate.

We conclude this section with two further brief developments concerning diagonalization of $\hat{H}(t)$ and $[\hat{H}(t)]^{\dagger}$. Consider the matrix $\Omega(t)$,

$$\Omega(t)=(\,|\,A_1(t)\rangle,|\,A_2(t)\rangle,\ldots) \tag{121}$$

which has columns made of the instantaneous kinematic eigenstates of $\hat{H}(t)$. Define also the matrix $\bar{\Omega}(t)$,

$$\bar{\Omega}(t)=(\,|\,\bar{A}_1(t)\rangle,|\,\bar{A}_2(t)\rangle,\ldots)\ , \tag{122}$$

which has columns made of the instantaneous kinematic eigenstates of $[\hat{H}(t)]^{\dagger}$. The orthonormality imposed in Eq. (32) yields

$$\bar{\Omega}^{\dagger}\Omega=\Omega\bar{\Omega}^{\dagger}=1\ . \tag{123}$$

Furthermore, the diagonal matrices of eigenvalues of $\hat{H}$ and $\hat{H}^{\dagger}$, respectively, Λ and Λ^*, are easily found as follows:

$$\Lambda=\bar{\Omega}^{\dagger}\hat{H}\Omega \tag{124}$$

and

$$\Lambda^*=\Omega^{\dagger}\hat{H}^{\dagger}\bar{\Omega}\ . \tag{125}$$

If $\hat{H}$ is symmetric, essentially the case in the rotating-wave approximation,

$$\hat{H}\,|\,A_r(t)\rangle=\lambda_r(t)\,|\,A_r(t)\rangle \tag{126}$$

$$=\hat{H}^{T}\,|\,A_r(t)\rangle \tag{127}$$

so that, by complex conjugation,

$$\hat{H}^{\dagger}(t)\,|\,A_r(t)\rangle^{*}=\lambda_r^{*}(t)\,|\,A_r(t)\rangle^{*}\ . \tag{128}$$

We thus learn that the entries in the column-vector representation for eigenstates of $\hat{H}^{\dagger}$ are just the complex conjugates of the corresponding ones for the associated eigenstates of $\hat{H}$. In this case

$$\overline{\Omega}=\Omega^{*}\ . \tag{129}$$

Finally, because of the importance of relating correctly normalized kinematic eigenstates at different times, we note that those at time $t_0<t_1$ are related to those of time t_1 simply by applying the operator

$$\tilde{\Omega}(t_1,t_0)=\sum_r\,|\,A_r(t)\rangle\langle\overline{A}_r(t_0)\,|\ . \tag{130}$$

Likewise, the operator

$$\tilde{\overline{\Omega}}(t_1,t_0)=\sum_r\,|\,\overline{A}_r(t_1)\rangle\langle A_r(t_0)\,| \tag{131}$$

relates $|\,\overline{A}_r(t_0)\rangle$ to $|\,A_r(t_1)\rangle$. That is,

$$|\,A_r(t_1)\rangle=\tilde{\Omega}(t_1,t_0)\,|\,A_r(t_0)\rangle \tag{132}$$

and

$$|\,\overline{A}_r(t_1)\rangle=\tilde{\overline{\Omega}}(t_1,t_0)\,|\,\overline{A}_r(t_0)\rangle\ . \tag{133}$$

Note that

$$\tilde{\Omega}(t_2,t_1)\tilde{\Omega}(t_1,t_0)=\tilde{\Omega}(t_2,t_0) \tag{134}$$

and

$$\tilde{\overline{\Omega}}(t_2,t_1)\tilde{\overline{\Omega}}(t_1,t_0)=\tilde{\overline{\Omega}}(t_2,t_0)\ . \tag{135}$$

For example, if $t_0=t_i$, $|\,\overline{A}_r(t_i)\rangle=|\,A_r(t_i)\rangle=|\,a_r\rangle$, we find the matrix elements relative to the $|\,a_r\rangle$ basis easily:

$$\tilde{\Omega}_{s',s}(t)=\langle a_s'\,|\,\tilde{\Omega}(t,t_i)\,|\,a_s\rangle=\langle a_s'\,|\,A_s(t)\rangle\ , \tag{136}$$

simply the s' component of the kinematic eigenstate $|\,A_s\rangle$. Thus with respect to the H_0-diagonal basis,

$$\tilde{\Omega}(t)=\Omega\ . \tag{137}$$

Similarly, one finds in this basis

$$\tilde{\overline{\Omega}}(t)=\overline{\Omega}\ . \tag{138}$$

VII. SUMMARY AND CONCLUSIONS

We have reexamined the conventional definition of nonionization (nondecay) probability as a norm of a state when the state evolves under an effective, non-Hermitian Hamiltonian $\hat{H}$. We have proceeded by first considering carefully the derivation of $\hat{H}$ and also of its Hermitian conjugate $\hat{H}^{\dagger}$. In Sec. II this analysis reveals that the eigenstates $|\,A\rangle$ of $\hat{H}$ are incoming scattering states projected onto the discrete subspace of bound states. The eigenstates $|\,\overline{A}\rangle$ of $\hat{H}^{\dagger}$ are found to be outgoing scattering states projected onto the bound-state subspace.

Similar considerations in Sec. III on the time-dependent Schrödinger equation lead to two time-dependent equations involving $\hat{H}$ and $\hat{H}^{\dagger}$. The operator $\hat{H}$ determines dynamic states $|\,\phi\rangle$ evolving into the future according to Eq. (54). These states are Schrödinger-picture incoming scattering states projected onto the bound-state subspace. In general, they are to be required to satisfy an initial-state condition, as specified by Eq. (56′). The operator $\hat{H}^{\dagger}$ determines dynamic states $|\,\overline{\phi}\rangle$ retroevolving from the future according to Eq. (55). These states are Schrödinger-picture outgoing scattering states projected onto the bound-state subspace. In general, they are to be required to fit a final-state condition, as specified in Eq. (57′).

It is convenient to impose a constant biorthonormality on the kinematic states $|\,A\rangle$ and $|\,\overline{A}\rangle$, as expressed in Eq. (32). Completeness then takes the form expressed in Eq. (33). The kinematic states $|\,A\rangle$ and $|\,\overline{A}\rangle$ provide a convenient basis with respect to which to refer the dynamics of the ionizing system, as contained in the evolution of the states $|\,\phi\rangle$ and $|\,\overline{\phi}\rangle$.

In Sec. IV we employ the S-matrix aspect of the dynamic projected states $|\,\phi\rangle$ and $|\,\overline{\phi}\rangle$, as revealed in the analysis of Secs. II and III, to construct transition matrix elements and occupation amplitudes within the bound-state subspace. The customary S matrix is defined in terms of remote past and future times. This leads in the adiabatic limit to the result (91). That is, each complex-energy mode attenuates exponentially and independently throughout the history of the interaction. It is crucial to note that this is possible *only if the decay rate of each mode is at all times proportional to its own occupation probability* since these rates are in principle all completely independent.

Our most significant results have to do with the interpolating, intermediate-time amplitudes and probabilities. We conveniently choose as a reference basis that set of states $\{\,|\,\overline{A}_r\rangle\}$ which adiabatically retroevolve from the asymptotically noninteracting (future) basis $|\,a_r\rangle$. The intermediate-time occupation probability of a state which evolves adiabatically into an arbitrary final state $|\,f\rangle$ is given by Eq. (64). For the general superposition state $|\,f\rangle$ this probability will exhibit oscillations. The total intermediate-time bound-state probability $P_B(t)$ is given by Eq. (65). This result should be independent of the fact that we have used an adiabatic reference basis. In contrast to the traditional norm-of-states definition of $P_B(t)$, the expression in (65) will not oscillate in time. These definitions of intermediate-time probabilities, dictated by S-matrix considerations, lead to the sensible result that $P_B(t)$ is at all times the sum of occupation probabilities of individual complex-energy eigenmodes.

The possibility of prescribing in a formal way a measure of intermediate-time occupation probabilities, as in Eq. (64), is of course attractive. It is also an attractive feature of our definition that $P_B(t)$ is given simply as a sum of individual-mode probabilities. Ultimately, however, a stronger argument is desirable. We believe the following consideration is unambiguous in its implications.

As noted above, a satisfactory definition of occupation probabilities for intermediate times must in the adiabatic limit exhibit the property that, *at all times,* the loss rate from each mode must be proportional to the instantaneous probability only of that (independent) mode. It is exactly this independent decay exhibited in the adiabatic limit in Eq. (90). The norm-of-state probability does not attenuate throughout the history of an interaction consistently with this result. [See, by contrast, Eq. (16) in AB and the time derivatives thereof. The nonzero overlap of eigenstates of $\hat{H}(t)$ would make asymptotic independent-exponential modal decays a very fortuitous situation.]

We call attention to the fact that our definition of intermediate-time probabilities is in contrast to the conventional prescription set forth by Lee, Ohme, and Yang.[11] We believe the reason that these authors adopted their particular prescription is that, in the context of only K-meson decays, one would not naturally be led to consider the S-matrix aspects of the problem. Such a situation, with switchable decay to a continuum, is much more plausible in the context of multiphoton ionization processes. It is only in an adiabatic limit with a switchable interaction that one might naturally consider both an S matrix and an intermediate-time occupation probability for complex-energy eigenmodes. Only then does the reconciliation of the asymptotic independent-exponential decay with intermediate-time probabilities compel one to seek an alternative to norm of state $P_B(t)$. It is only in the context of the S-matrix aspect of effective Hamiltonians that it is likely to be realized that occupation probabilities are to be constructed with evolved *and* retroevolved states. *The norm-of-state definition is essentially equivalent to trying to form $P_B(t)$ as a norm of an incoming state.*

The effective, time-dependent Schrödinger equation pair, (54) and (55), together with the initial- and final-state conditions (56) and (57) and the definition of probabilities in Eq. (64), represent a kind of generalization of quantum dynamics to non-Hermitian systems. On a discrete basis of ionizing states, this formalism represents a convenient approach to calculating individual occupation probabilities, total bound-state probability, and instantaneous loss rate. Of course, it is necessary that the time intervals under consideration be short enough that the coherence of the state of the system not be destroyed by such phase-shifting processes as spontaneous emission, collisions, etc. In such situations, however, a generalized density-matrix formalism can be employed. For K-meson decays these phase-shifting processes are less of a problem.

For completeness we have considered the resolvent operator for a non-Hermitian dynamical system in Sec. VI. The resolvent formalism is applicable during time intervals when the interaction varies insignificantly. Time-translation operators T_i and T_f are obtained as Fourier transforms of the resolvent. These satisfy a simple semigroup property. We emphasize that the conventional states of unit norm, such as are suitable for Hermitian dynamics, are *not* a satisfactory basis when the interaction is non-Hermitian. We point out that for symmetric $\hat{H}$, either $\hat{H}$ or $\hat{H}^\dagger$ may be easily diagonalized by a similarity transformation. The appropriate transformations are provided in general, in a simple form.

Finally, in the Appendix, we illustrate our considerations on the general non-Hermitian $\hat{H}$ for a two-state system. Solutions are obtained for the time-dependent Schrödinger equations by extending the Payne-Choi scheme to accommodate arbitrary initial- and final-state conditions. The instantaneous kinematic eigenstates of $\hat{H}$ are also obtained by following the procedure defined by Armstrong and Baker. The decay rates in either approach agree to all orders in $\hat{H}$. It is noteworthy that the kinematic states evolved as solutions to the time-dependent Schrödinger equations automatically incorporate the orthonormality conditions. This normalization, of course, must be implemented by hand when computing the eigenstates by solving the eigenvalue equation. This model also makes graphically clear the contrast between a norm-of-states definition of probabilities and the S-matrix determined, interpolating ones we have identified. In this two-state model a norm-of-states definition of $P_B(t)$ leads to extra influences on occupation probabilities through normalization-of-states effects, in addition to the exponential decay. These extra effects have no obvious physical interpretation. Also, the intrinsic S-matrix aspects of effective-Hamiltonian formalisms makes clear the origin of the automatic biorthonormality of the dynamic states evolved by the Schrödinger equations. We compute the nature of the overlap of the eigenstates for a special case, which is manifestly nonzero according to the requirement of "all orders in resonance transitions, first order in decay rates." Finally, we compute the resolvent operator for this general model, which is then used to construct explicitly the time-translation operators.

The theory of non-Hermitian quantum dynamics, as we have inferred it from its basis in scattering theory, makes predictions of intermediate-time occupation probabilities which are quite different from the conventional norm-of-state construction. The possibility of multiphoton ionization of systems through near-resonant intermediate states, as well as the decay of degenerate coupled states such as the K_0 mesons, makes such a theory nonacademic, and even essential to a correct analysis. In the case of multiphoton ionization on resonance, a generalization of the present formalism in terms of a density matrix would be required. On resonance the adiabatic limit also is irrelevant. However, for the K_0-meson decays, the present formalism seems quite appropriate. The theoretical ground is rich for further studies, and their relevance to experiment seems apparent.

APPENDIX

1. General two-state non-Hermitian system

We wish to consider here in detail the dynamics of a general two-state non-Hermitian system. This system provides all essential elements to illustrate the features of the general problem.

We consider the most general non-Hermitian 2×2 Hamiltonian matrix, $\hat{H}(t)$. However, we shall obtain the time-dependent solution in the adiabatic limit. The technique by which this is accomplished is an adiabatic iterative technique developed by Choi and Payne,[3] although we

carry the solution further, to incorporate arbitrary initial superposition states. We obtain solutions satisfying not only the incoming Schrödinger equation [Eq. (54)] subject to the initial-state condition Eq. (56), but also solutions satisfying the outgoing Schrödinger equation [Eq. (55)] satisfying the final-state condition Eq. (57).

Next, we follow the procedure of finding directly the kinematic states of $\hat{H}(t)$, that is, instantaneous eigenstates. According to our theory, the imaginary parts of the complex-energy eigenvalues are identified as decay half-widths. The results agree fully with the explicit time-dependent solutions obtained in the adiabatic limit.

Third, we compute the overlap between the two kinematic eigenstates and find that, considered to all orders in the resonance-transition matrix elements, and to first order in the decay terms, there is a nonvanishing contribution. Thus for initial superposition states there are important differences between our construction of transition amplitudes and occupation probabilities, with non-Hermitian Hamiltonians, and that of conventional quantum mechanics with Hermitian Hamiltonians.

Finally, we calculate the resolvent operator for this system. Of course, it is found to have poles at the same complex-energy values of the two other calculations. The time-translation operators are obtained explicitly, and the property of closure is illustrated with the kinematic eigenstates.

The Hamiltonian we shall investigate is expressed as

$$\hat{H}(t)=\begin{bmatrix}\delta(t)-\dfrac{i\gamma_2(t)}{2} & -v(t)\\ -u(t) & \dfrac{-i\gamma_1(t)}{2}\end{bmatrix}. \tag{A1}$$

All entries are permitted to be time dependent, either because of an assumed "switching," or time-profile function, or because the interaction is included as a semiclassical one. Time-dependent Stark shifts are included in the time-dependent "detuning" $\delta(t)$. We shall assume $\delta(t)$ is "small," so that near-resonance obtains, but shall avoid the situation of exact resonance. We define the general time-dependent states as

$$|\phi(t)\rangle=\begin{bmatrix}a_2(t)\\ a_1(t)\end{bmatrix},\quad |\bar{\phi}(t)\rangle=\begin{bmatrix}\bar{a}_2(t)\\ \bar{a}_1(t)\end{bmatrix}. \tag{A2}$$

The time-dependent Schrödinger equations (54) and (55) give

$$i\dot{a}_2=\left[\delta-\frac{i\gamma_2}{2}\right]a_2-va_1\,, \tag{A3}$$

$$i\dot{a}_1=-ua_2-\frac{i\gamma_1}{2}a_1\,, \tag{A4}$$

and

$$i\dot{\bar{a}}_2=\left[\delta+\frac{i\gamma_2}{2}\right]\bar{a}_2-u^*\bar{a}_1\,, \tag{A5}$$

$$i\dot{\bar{a}}_1=-v^*\bar{a}_2+\frac{i\gamma_1}{2}\bar{a}_1\,. \tag{A6}$$

The eigenvalue equations (30) and (31) become

$$\begin{bmatrix}\delta-\dfrac{i\gamma_2}{2} & -v\\ -u & \dfrac{-i\gamma_1}{2}\end{bmatrix}\begin{bmatrix}a_2(t)\\ a_1(t)\end{bmatrix}=\lambda(t)\begin{bmatrix}a_2(t)\\ a_1(t)\end{bmatrix} \tag{A7}$$

and

$$\begin{bmatrix}\delta+\dfrac{i\gamma_2}{2} & -u^*\\ -v^* & \dfrac{-\gamma_1}{2}\end{bmatrix}\begin{bmatrix}\bar{a}_2(t)\\ \bar{a}_1(t)\end{bmatrix}=\lambda^*(t)\begin{bmatrix}\bar{a}_2(t)\\ \bar{a}_1(t)\end{bmatrix}. \tag{A8}$$

Anticipating solutions $\lambda_\pm(t)$ of (A7) and $\lambda_\pm^*(t)$ of (A8), we define the associated orthonormal (kinematic) basis sets, satisfying (32), as

$$|A_+(t)\rangle=\begin{bmatrix}a_{2+}(t)\\ a_{1+}(t)\end{bmatrix},\quad |A_-(t)\rangle=\begin{bmatrix}a_{2-}(t)\\ a_{1-}(t)\end{bmatrix}, \tag{A9}$$

and

$$|\bar{A}_+(t)\rangle=\begin{bmatrix}\bar{a}_{2+}(t)\\ \bar{a}_{1+}(t)\end{bmatrix},\quad |\bar{A}_-(t)\rangle=\begin{bmatrix}\bar{a}_{2-}(t)\\ \bar{a}_{1-}(t)\end{bmatrix}. \tag{A10}$$

These are to satisfy

$$\bar{a}^*_{2+}a_{2+}+\bar{a}^*_{1+}a_{1+}=1\,, \tag{A11}$$

$$\bar{a}^*_{2-}a_{2-}+\bar{a}^*_{1-}a_{1-}=1\,, \tag{A12}$$

and

$$\bar{a}^*_{2+}a_{2-}+\bar{a}^*_{2+}a_{1-}=0\,, \tag{A13}$$

$$\bar{a}^*_{2-}a_{2+}+\bar{a}^*_{1-}a_{2-}=0\,. \tag{A14}$$

In solving for amplitudes satisfying (A7) and (A8), the results of Eqs. (A13) and (A14) will obtain automatically. However, Eqs. (A11) and (A12) must be imposed. Part of the problem of interpretation of non-Hermitian dynamics has to do with the physical significance of the mathematical possibility of this imposed orthonormality. As will be seen, it is a natural dynamical consequence of the Schrödinger equation.

A cautionary note is in order. The amplitudes appearing in Eqs. (A3)—(A6) are dynamically evolved amplitudes. In general, they will be attenuated relative to the kinematic amplitudes defined in Eqs. (A7)—(A14). The proper distinctions will be drawn when necessary.

Finally, we shall express the complex-energy eigenvalues in the form of a purely real part $\epsilon(t)$, and another purely real part $\gamma(t)$, in the form

$$\lambda_\pm(t)=\epsilon_\pm(t)-i\frac{\gamma_\pm}{2}(t)\,. \tag{A15}$$

2. Time-dependent Schrödinger equations

In order to solve the dynamical equations (A3) and (A4), we define new amplitudes related to $a_1(t)$ and $a_2(t)$ as follows:

$$A_1(t)=a_1(t)\exp\left[\int_{t_1}^{t}\tfrac{1}{2}\gamma_1(t')dt'\right]$$
$$A_2(t)=a_2(t)\exp\left[i\int_{t_i}^{t}[\delta(t')-\tfrac{1}{2}i\gamma_1(t')]dt'\right]. \quad \text{(A16)}$$

The equations of motion become

$$\frac{dA_2}{dt}=\frac{\gamma_1-\gamma_2}{2}A_2+iv\exp\left[i\int_{t_i}^{t}\delta(t')dt'\right]A_1 \quad \text{(A17)}$$

$$\equiv-\gamma A_2+iv\exp\left[i\int_{t_i}^{t}\delta(t')dt'\right]A_1 \quad \text{(A18)}$$

and

$$\frac{dA_1}{dt}=iu\exp\left[-i\int_{t_i}^{t}\delta(t')dt'\right]A_2 . \quad \text{(A19)}$$

We may eliminate A_1 in Eq. (A18) by using (A19):

$$\frac{d^2A_2}{dt^2}+\left[\gamma-\frac{d\ln v}{dt}-i\delta\right]\frac{dA_2}{dt}+\left[uv+\frac{d\gamma}{dt}-\gamma\frac{d\ln v}{dt}-i\gamma\delta\right]A_2=0 , \quad \text{(A20a)}$$

$$\left[\frac{d}{dt}+h_1\right]\left[\frac{d}{dt}+h_2\right]A_2=0 \quad \text{(A20b)}$$

and find from Eq. (A20)

$$h_1+h_2=\gamma-i\delta-\frac{d\ln v}{dt} , \quad \text{(A21)}$$

$$\frac{dh_2}{dt}+h_1h_2=uv-i\delta\gamma+\frac{d\gamma}{dt}-\gamma\frac{d\ln v}{dt} . \quad \text{(A22)}$$

Consider now the time dependence of the quantities u, v, and $\gamma_{1,2}$ in terms of a specific switching function, or envelope function, $\eta(t)$. Representing any of u, v, or $\gamma_{1,2}$ by q, for the moment, let us write

$$q(t)=\eta(t)q(0) . \quad \text{(A23)}$$

As an example, let

$$\eta(t)=e^{-\alpha|t|} . \quad \text{(A24)}$$

Then, $\dot\eta=O(\alpha)$, $\ddot\eta=O(\alpha^2)$, $\dot\eta\ddot\eta=O(\alpha^3)$, etc. Following Choi and Payne,[3] one now solves (A21) and (A22) to zeroth order in α by neglecting the derivative term. Next, this zeroth-order solution gives in (A22) a first-order correction term in the derivative. The process can be iterated. To leading correction terms in α, one obtains, after some tedious algebra and carefully incorporating initial-value considerations, the following results:

$$h_2=-\frac{i}{2}(\tilde\delta-\sigma\tilde\Omega)+\frac{1}{2}\frac{d}{dt}\ln\left[\frac{\sigma\tilde\Omega}{\tilde\delta^*+\sigma\tilde\Omega}\right] , \quad \text{(A25)}$$

and

$$h_1=-\frac{i}{2}(\tilde\delta+\sigma\tilde\Omega)-\frac{1}{2}\frac{d}{dt}\ln\left[\frac{\eta^2\sigma\tilde\Omega}{\tilde\delta^*+\sigma\tilde\Omega}\right] . \quad \text{(A26)}$$

We have defined

$$\sigma=\mathrm{sgn}\delta , \quad \text{(A27)}$$
$$\tilde\delta=\delta+i\gamma , \quad \text{(A28)}$$

and

$$\tilde\Omega^2=\tilde\delta^{*2}+4uv . \quad \text{(A29)}$$

We find the general solution of Eq. (A20) in the form

$$A_2(t)=A_2(t_i)\exp\left[-\int_{t_i}^{t}h_2(t')dt'\right]+\frac{iV(t_i)A_1(t_i)}{h_2(t)-h_1(t)}\exp\left[-\int_{t_i}^{t}h_1(t')dt'\right] . \quad \text{(A30)}$$

Certain terms have been omitted because they will eventually vanish with $\eta(t_i)=0$. The results Eqs. (A25) and (A26) may be used in (A30), and performing the integrations, involving the total-derivative terms, yields the result

$$A_2(t)=A_2(t_i)\left[\frac{1}{2}\left[1+\frac{\sigma\tilde\delta^*}{\tilde\Omega}\right]\right]^{1/2}\exp\left[\tfrac{1}{2}\int_{t_i}^{t}(\tilde\delta-\sigma\tilde\Omega)dt'\right]+\frac{A_1(t_i)}{\tilde\Omega}\frac{\sigma v(t)}{\left[\frac{1}{2}\left[1+\frac{\sigma\tilde\delta^*}{\tilde\Omega}\right]\right]^{1/2}}\exp\left[\tfrac{1}{2}\int_{t_i}^{t}(\tilde\delta+\sigma\tilde\Omega)dt'\right] . \quad \text{(A31)}$$

This result may in turn be employed in (A19), and integration by parts yields the result

$$A_1(t)=-\frac{A_2(t_i)}{\tilde\Omega}\frac{\sigma u}{\left[\frac{1}{2}\left[1+\frac{\sigma\tilde\delta^*}{\tilde\Omega}\right]\right]^{1/2}}\exp\left[-\frac{i}{2}\int_{t_i}^{t}(\tilde\delta^*+\sigma\tilde\Omega)dt'\right]+A_1(t_i)\left[\frac{1}{2}\left[1+\frac{\sigma\tilde\delta^*}{\tilde\Omega}\right]\right]^{1/2}\exp\left[-\frac{i}{2}\int_{t_i}^{t}(\tilde\delta^*-\sigma\tilde\Omega)dt'\right] . \quad \text{(A32)}$$

Recalling now the definitions (A16), and defining

$$2\lambda_{\pm}=\delta-\frac{i(\gamma_2+\gamma_1)}{2}\pm\sigma\tilde{\Omega}\ , \tag{A33}$$

the results (A31) and (A32) may be expressed in the form

$$|\phi_i(t)\rangle=a_2(t_i)\,|A_+(t)\rangle\exp\left[-i\int_{t_i}^{t}\lambda_+(t')dt'\right] +a_1(t_i)\,|A_-(t)\rangle\exp\left[-i\int_{t_i}^{t}\lambda_-(t')dt'\right], \tag{A34}$$

where we have defined kinematic states $|A_+\rangle$ and $|A_-\rangle$ as

$$|A_+(t)\rangle=\begin{bmatrix}\left[\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]\right]^{1/2}\\ \frac{\sigma u}{\tilde{\Omega}\left[\frac{1}{2}\left[1+\sigma\frac{\tilde{\delta}^*}{\tilde{\Omega}}\right]\right]^{1/2}}\end{bmatrix}, \tag{A35}$$

$$|A_-(t)\rangle=\begin{bmatrix}\frac{\sigma v}{\tilde{\Omega}\left[\frac{1}{2}\left[1+\sigma\frac{\tilde{\delta}^*}{\tilde{\Omega}}\right]\right]^{1/2}}\\ \left[\frac{1}{2}\left[1+\sigma\frac{\tilde{\delta}^*}{\tilde{\Omega}}\right]\right]^{1/2}\end{bmatrix}. \tag{A36}$$

Because we have

$$\lim_{t\to t_i}|A_+(t)\rangle=\begin{bmatrix}1\\0\end{bmatrix} \tag{A37}$$

and

$$\lim_{t\to t_i}|A_-(t)\rangle=\begin{bmatrix}0\\1\end{bmatrix}, \tag{A38}$$

our general solution Eq. (A34) automatically incorporates the arbitrary initial condition

$$\lim_{t\to t_i}|\phi_i(t)\rangle=\begin{bmatrix}a_2(t_i)\\a_1(t_i)\end{bmatrix}. \tag{A39}$$

The solutions to Eqs. (A5) and (A6) are obtained in a similar manner. The important difference is that we should require a final-state condition in our solution:

$$\lim_{t\to t_f}|\bar{\phi}_f(t)\rangle=\begin{bmatrix}a_2(t_f)\\a_1(t_f)\end{bmatrix}. \tag{A40}$$

Following procedures similar to before, we now find the result

$$|\bar{\phi}_f(t)\rangle=a_2(t_f)\,|\bar{A}_+(t)\rangle\exp\left[-i\int_{t_f}^{t}\lambda_+^*(t')dt'\right] +a_1(t_f)\,|\bar{A}_-(t)\rangle \times\exp\left[-i\int_{t_f}^{t}\lambda_-^*(t')dt'\right], \tag{A41}$$

where here

$$|\bar{A}_+(t)\rangle=\begin{bmatrix}\left[\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]\right]^{1/2}\\ \frac{-\sigma v^*}{\tilde{\Omega}^*\left[\frac{1}{2}\left[1+\frac{\sigma\delta}{\tilde{\Omega}^*}\right]\right]^{1/2}}\end{bmatrix} \tag{A42}$$

and

$$|\bar{A}_-(t)\rangle=\begin{bmatrix}\frac{\sigma u^*}{\tilde{\Omega}^*\left[\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]\right]^{1/2}}\\ \left[\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]\right]^{1/2}\end{bmatrix}. \tag{A43}$$

It is readily checked that the orthonormality conditions (A11)—(A14) have been automatically included, in these kinematic-state coefficients of the exponentials, by the Schrödinger equations. For example,

$$\langle A_+(t)\,|\,\bar{A}_+(t)\rangle=\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]+\frac{u^*v^*}{\tilde{\Omega}^{*2}\frac{1}{2}\left[1+\sigma\frac{\tilde{\delta}}{\tilde{\Omega}^*}\right]} \tag{A44}$$

$$=\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]+\frac{1-\frac{\tilde{\delta}^2}{\tilde{\Omega}^{*2}}}{2\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]} \tag{A45}$$

$$=1\ . \tag{A46}$$

In the second step we have used the definition (A29). Also notice that if we had imposed initial-state conditions on the solution (A41) at an earlier time t_i, these states would increase exponentially in time. The natural orthonormality and the time behavior (A41) seem to be strong support for our overall theory of ionization and decay. Without the general consideration made in the general framework of S-matrix theory, these results would be meaningless curiosities.

Finally, the physical decay rates are to be obtained by expanding the eigenvalues $\lambda_{\pm}$ in (A33) to first order in γ's. We obtain, finally,

$$2\lambda_{\pm}=\delta\pm\sigma\Omega-i\left[1\mp\frac{\sigma\delta}{\Omega}\right]\frac{\gamma_1}{2}-i\left[1\pm\frac{\sigma\delta}{\Omega}\right]\frac{\gamma_2}{2}\ , \tag{A47}$$

where here

$$\Omega^2=\delta^2+4uv\ . \tag{A48}$$

The imaginary parts of the complex energies, to first order in $\gamma_{1,2}$, are thus

$$\frac{\gamma_{\pm}}{2}=\left[1\mp\frac{\sigma\delta}{\Omega}\right]\frac{\gamma_1}{4}+\left[1\pm\frac{\sigma\delta}{\Omega}\right]\frac{\gamma_2}{4}\ . \tag{A49}$$

To zeroth order in $\gamma_{1,2}$ we also find

$$\bar{a}^*_{2\pm}a_{2\pm}=\frac{1}{2}\left[1\pm\frac{\sigma\delta}{\Omega}\right], \tag{A50}$$

$$\bar{a}^*_{1\pm}a_{1\pm}=\frac{1}{2}\left[1\mp\frac{\sigma\delta}{\Omega}\right]. \tag{A51}$$

Therefore, (A49) may be expressed in the form

$$\gamma_\pm=\bar{a}^*_{2\pm}a_{2\pm}\gamma_2+\bar{a}^*_{1\pm}a_{1\pm}\gamma_1 . \tag{A52}$$

3. Kinematic eigenstates

We want to show now that the procedure of finding instantaneous eigenstates of $\hat{H}$ and $\hat{H}^\dagger$, with suitable normalization, leads to the same kinematic eigenstates as are naturally introduced by the time-dependent effective Schrödinger equations. In the adiabatic limit these eigenstates will be dynamically evolved from initial eigenstates of H_0 according to our discussion in Sec. V. Of course, the dynamical eigenstates will carry attenuated amplitude coefficients relative to the kinematic states which have constant orthonormality constraints.

The eigenvalue problems to be solved are those expressed in Eqs. (A7) and (A8). The secular equation is

$$\begin{vmatrix} \delta-\frac{i\gamma_2}{2}-\lambda & -v \\ -u & -\lambda-\frac{i\gamma_1}{2} \end{vmatrix}=0 . \tag{A53}$$

The solutions are readily found,

$$2\lambda_\pm=\delta-\tfrac{1}{2}i(\gamma_1+\gamma_2) \pm\sigma\{[\delta+i(\gamma_1-\gamma_2)]^2+4uv\}^{1/2}, \tag{A54}$$

and using (A28) and (A29) are seen to be the same as defined in (A33).

These may now be used in the eigenvalue equations (A7) and (A8) to determine the eigenamplitudes. For $\lambda_\pm$ we obtain the relationships

$$a_{2\pm}=\frac{2v}{\tilde{\delta}^*\mp\sigma\tilde{\Omega}}a_{1\pm} , \tag{A55}$$

and for $\lambda^*_\pm$

$$\bar{a}_{2\pm}=\frac{2u^*}{\tilde{\delta}\mp\tilde{\sigma}\tilde{\Omega}^*}a_{1\pm} . \tag{A56}$$

At this juncture one must impose some normalization conditions. Our general considerations lead us to impose those of (A11) and (A12). With (A55) and (A56) we find the results

$$\bar{a}^*_{1\pm}a_{1\pm}=\frac{1}{2}\left[1\mp\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right], \tag{A57}$$

$$\bar{a}^*_{2\pm}a_{2\pm}=\frac{1}{2}\left[1\pm\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]. \tag{A58}$$

It is readily checked that (A13) and (A14) are automatically satisfied.

Finally, one must choose a set of amplitudes that satisfy Eqs. (A55) and (A56). One finds easily that the kinematic eigenstates (A35) and (A36), and (A42) and (A44), evolved by the time-dependent Schrödinger equation satisfy these equations. Therefore, there is complete agreement in the two approaches, providing the instantaneous eigenstates are appropriately normalized and that appropriate initial- and final-state conditions are imposed on the dynamical solutions to the time-dependent Schrödinger equations. Again, physical decay rates (first order in $\gamma_{1,2}$) are obtained by expanding (A54), leading of course to the original result (A52) of the time-dependent calculation.

4. Overlap

We wish to obtain here the overlap between the two kinematic eigenstates $|A_+\rangle$ and $|A_-\rangle$ for our model non-Hermitian Hamiltonian. Because of the possibility of non-negligible overlap between different eigenstates of $\hat{H}$, the norm-of-state bound-state probability definition predicts a decay pattern which oscillates between the frequencies of the two eigenmodes of complex energies whenever one has an initial state that is a superposition of eigenstates of $\hat{H}(t)$.

As the simplest possible example, let us set $u^*=u=v$ in our model Hamiltonian $\hat{H}$ in (A1). With the use of the expressions (A35) and (A36),

$$\langle A_+|A_-\rangle=\frac{\sigma v}{\tilde{\Omega}}\left[\frac{1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}}}{1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}}\right]^{1/2}-\frac{\sigma v}{\tilde{\Omega}^*}\left[\frac{1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}}{1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}}\right]^{1/2} \tag{A59}$$

$$=2i\sigma v\,\mathrm{Im}\left[\frac{1}{\tilde{\Omega}}\right]\times\left[\left[1+\frac{\sigma\tilde{\delta}}{\tilde{\Omega}^*}\right]\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]^{-1}\right]^{1/2} . \tag{A60}$$

Expanding the expression (A29) for $\tilde{\Omega}$ and defining Ω as in (A48),

$$\tilde{\Omega}\cong\Omega-\frac{i\delta}{2\Omega}(\gamma_2-\gamma_1) . \tag{A61}$$

Finally, therefore,

$$\langle A_+|A_-\rangle\cong\frac{iv}{\Omega^2}(\gamma_2-\gamma_1) . \tag{A62}$$

Considered to all orders in the resonance-transition matrix elements u and v, and to first order in $\gamma_{1,2}$, the overlap is not negligible.

5. Closure and the resolvent

With the kinematic eigenstates (A35) and (A36), and (A42) and (A43), it is a simple matter to illustrate closure. Closure is obtained as follows:

$$|A_+\rangle\langle\bar{A}_+|+|A_-\rangle\langle\bar{A}_-|=\begin{bmatrix}\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right] & -\frac{\sigma v}{\tilde{\Omega}} \\ -\frac{\sigma u}{\Omega} & \frac{uv}{\tilde{\Omega}\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]}\end{bmatrix}+\begin{bmatrix}\frac{uv}{\tilde{\Omega}\frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]} & \frac{\sigma v}{\tilde{\Omega}} \\ \frac{\sigma u}{\tilde{\Omega}} & \frac{1}{2}\left[1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\right]\end{bmatrix}$$

$$=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}. \tag{A63}$$

Use has been made again of (A29). Defining projection operators

$$P_+=|A_+\rangle\langle\bar{A}_+|,\quad P_-=|A_-\rangle\langle\bar{A}_-|\ , \tag{A64}$$

(A63) is simply the statement that

$$P_++P_-=P_+^++P_-^+=1\ . \tag{A65}$$

To obtain the resolvent, for $\hat{H}$ for example, we must solve the equation

$$(Z-\hat{H})G_i(z)=\begin{bmatrix}z-\delta+\frac{i\gamma_2}{2} & v\\ u & z+\frac{i\gamma_1}{2}\end{bmatrix}\begin{bmatrix}G_{11} & G_{21}\\ G_{12} & G_{11}\end{bmatrix}=1\ . \tag{A66}$$

The inversion is readily performed, yielding

$$G_i(z)=\frac{1}{(z-\lambda_+)(z-\lambda_-)}\begin{bmatrix}z+\frac{i\gamma_1}{2} & -v\\ -u & z-\delta+\frac{i\gamma_2}{2}\end{bmatrix}, \tag{A67}$$

where the $\lambda_\pm$ are the same as found in (A54) and (A47). For the time-translation operator we obtain

$$T_i(t-t_0)=\frac{1}{2\pi i}\int_{i\epsilon+\infty}^{i\epsilon-\infty}G(z)e^{-iz(t-t_0)} \tag{A68}$$

$$=\frac{1}{2}\begin{bmatrix}1+\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}} & \frac{-2\sigma v}{\tilde{\Omega}}\\ -2\sigma u & 1-\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\end{bmatrix}e^{-i\lambda_+(t-t_0)}\Theta(t-t_0)-\frac{1}{2}\begin{bmatrix}1-\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}} & -\frac{2\sigma v}{\tilde{\Omega}}\\ -\frac{2\sigma u}{\tilde{\Omega}} & -1-\frac{\sigma\tilde{\delta}^*}{\tilde{\Omega}}\end{bmatrix}e^{-i\lambda_-(t-t_0)}\Theta(t-t_0)\ . \tag{A69}$$

This may be written in terms of the projectors $P_\pm$ as

$$T_i(t-t_0)=\Theta(t-t_0)(P_+e^{-i\lambda_+(t-t_0)}+P_-e^{-i\lambda_-(t-t_0)})\ . \tag{A70}$$

In a similar manner one finds, for the reverse-time translation operator for $\hat{H}^\dagger$,

$$T_f(t-t_f)=\Theta(t_f-t)(P_+^+e^{-i\lambda_+^*(t-t_f)}+P_-^+e^{-i\lambda_-^*(t-t_f)})\ . \tag{A71}$$

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