PHYSICAL REVIEW A VOLUME 28, NUMBER 6 DECEMBER 1983

Unitarity, the pole approximation, and interference between radiative emission and autoionization

S. L. Haan and J. Cooper

Joint Institute for Laboratory Astrophysics, University of Colorado and National Bureau of Standards, Boulder, Colorado 80309

(Received 12 July 1983)

In model problems involving the "decay" of discrete states into electron and photon continua there is frequently a final-state coupling between the two continua which must be considered. Armstrong, Theodosiou, and Wall have shown that this coupling can change the relative decay probabilities into the two channels. We examine and interpret this continuum-continuum coupling further, paying particular attention to questions of unitarity violation and the validity of the pole or Markov approximation for the continuum-continuum coupling. We also examine unitarity violation and the pole approximation in a more general context, and discuss criteria under which the approximation can be made in sequential diagonalizations. Finally, we interpret the square of the Fano q value as the ratio of two rates in the pole approximation.

I. INTRODUCTION

In a 1978 paper, Armstrong, Theodosiou, and Wall[1] (ATW) considered several model problems involving the "decay" of discrete states into coupled free-electron and photon continua. In the simplest case they considered, a single discrete state (for example, an autoionizing state) lies embedded in a free-electron continuum, and both the discrete state and the continuum are assumed to be coupled to some (stable) final atomic state, and correspondingly to a photon continuum, by the vacuum fluctuations of the radiation field. For such a system, ATW showed that the continuum-continuum coupling can strongly affect the relative probabilities for obtaining an asymptotic electron or photon.

ATW also considered systems in which more than one discrete state was involved, and such model systems have recently been studied again by numerous authors in the context of laser-induced autoionization (hereafter LIA).[2] In particular Agarwal, Haan, Burnett, and Cooper,[3,4] Crance and Armstrong,[5] and Lewenstein, Haus, and Rzazewski[6] have all examined spontaneous radiative decay in LIA, and consequently within this context it is important to understand the nature and importance of spontaneous radiative decay from the electron continuum. The purpose of this work is to examine physical aspects of this continuum-continuum coupling and, more generally, to consider unitarity violation and the pole approximation.

II. EXACT SOLUTION FOR THE TWO-CONTINUUM SYSTEM

ATW denoted the eigenstates of the Hamiltonian H^0 describing the free-electron and photon continua by $\{|ie)\}$ and $\{|f\omega)\}$, respectively; e and ω represent the relevant energies of the decay product. The two continua are coupled by the matrix element $(ie|V|f\omega)=H_{e\omega}$ representing spontaneous radiative decay. ATW "diagonalize" the two-continuum system using the reaction or K matrix, which they define in an integral equation. However, a closed-form solution for the diagonalized continua can be obtained if one writes the continuum-continuum coupling in a separable form such as

$$H_{e\omega}=f^*(e)g(\omega) \tag{1}$$

for some $f(e)$ depending on electron energy and some $g(\omega)$ depending on photon frequency. For spontaneous radiative decay in the usual electric dipole approximation, $f(e)$ is essentially a dipole matrix element between the electron continuum and the final atomic state, while $g(\omega)$ includes the familiar $\omega^{3/2}$ factor and multiplicative algebraic factors.[7]

One method of diagonalization involves the Møller operator Ω_- of scattering theory.[4] Ω_- provides an isometric and invertible transformation from the continuum eigenstates of some Hamiltonian H^0 to the continuum eigenstates of the Hamiltonian $H=H^0+V$, provided the potential V satisfies the usual asymptotic conditions of scattering theory.[8] If $|e\}$ and $|\omega\}$ denote the diagonalized electron and photon continua, then[9]

$$\begin{aligned}|e\}&=\Omega_-|ie)\,,\\|\omega\}&=\Omega_-|f\omega)\,.\end{aligned} \tag{2}$$

The Møller operator can in turn be expressed in terms of the Green's operator, or resolvent,

$$G(z)=(z-H)^{-1}$$

to obtain

$$\begin{aligned}|e\}&=[1+G(e-i\epsilon)V]|ie)\,,\\|\omega\}&=[1+G(\omega-i\epsilon)V]|f\omega)\,,\end{aligned} \tag{3}$$

where the "$i\epsilon$" indicates the lim$\epsilon\downarrow 0$ is to be taken. Linear equations coupling the matrix elements of the resolvent can be obtained from the equation

$$(z-H^0)G(z)=1+VG(z)\,. \tag{4}$$

These equations are easily solved for the coupling (1), and formal expressions for $|e\}$ and $|\omega\}$ can then be obtained.

 ©1983 The American Physical Society

One finds

$$
\begin{aligned}
|e\} &= |ie) + \int d\omega \frac{|f\omega)g^*(\omega)}{e-i\epsilon-\omega}\,\frac{f(e)}{\psi(e-i\epsilon)} \\
&\quad + \int de' \frac{|ie')f^*(e')}{e-i\epsilon-e'}\,\frac{\Sigma^{gg}(e-i\epsilon)f(e)}{\psi(e-i\epsilon)}\,, \\
|\omega\} &= |f\omega) + \int de \frac{|ie)f^*(e)}{\omega-i\epsilon-e}\,\frac{g(\omega)}{\psi(\omega-i\epsilon)} \\
&\quad + \int d\omega' \frac{|f\omega')g^*(\omega')}{\omega-i\epsilon-\omega'}\,\frac{\Sigma^{ff}(\omega-i\epsilon)g(\omega)}{\psi(\omega-i\epsilon)}\,,
\end{aligned}
\tag{5a}
$$

where

$$\psi(z)=1-\Sigma^{ff}(z)\Sigma^{gg}(z)\,, \tag{5b}$$

$\Sigma(z)$ denotes matrix "self-energies"

$$\Sigma^{ff}(z)=\int de \frac{|f(e)|^2}{z-e}\,, \tag{6a}$$

$$\Sigma^{gg}(z)=\int d\omega \frac{|g(\omega)|^2}{z-\omega}\,. \tag{6b}$$

If some discrete state $|a\rangle$ is coupled to these continua by an interaction V, then

$$
\begin{aligned}
\langle a|V|e\} &= \langle a|V|ie) + \frac{\Sigma^{ag}(e-i\epsilon)f(e)}{\psi(e-i\epsilon)} \\
&\quad + \frac{\Sigma^{af}(e-i\epsilon)\Sigma^{gg}(e-i\epsilon)f(e)}{\psi(e-i\epsilon)}\,,
\end{aligned}
\tag{7a}
$$

$$
\begin{aligned}
\langle a|V|\omega\} &= \langle a|V|f\omega) + \frac{\Sigma^{af}(\omega-i\epsilon)g(\omega)}{\psi(\omega-i\epsilon)} \\
&\quad + \frac{\Sigma^{ag}(\omega-i\epsilon)\Sigma^{ff}(\omega-i\epsilon)g(\omega)}{\psi(\omega-i\epsilon)}\,,
\end{aligned}
\tag{7b}
$$

where

$$\Sigma^{ag}(z)=\int d\omega \frac{\langle a|V|f\omega)g^*(\omega)}{z-\omega}\,,$$

$$\Sigma^{af}(z)=\int de \frac{\langle a|V|ie)f^*(e)}{z-e}\,.$$

If desired one can make the Markov or pole approximation (PA) on the self-energies by using

$$\frac{1}{E-E'\pm i\epsilon}=\mathrm{P}\left[\frac{1}{E-E'}\right]\mp i\pi\delta(E-E') \tag{8}$$

and keeping only the δ function part of each integral in the self-energy definitions. This approximation should be valid over a wide range of the continua if $\langle a|V|f\omega)$, $\langle a|V|ie)$, $f(e)$, and $g(\omega)$ vary slowly and smoothly with energy; the approximation would clearly be invalid close to threshold or very far into the continuum where the integrand of the principal-value integral is very asymmetric about $E=E'$.

III. BRANCHING RATIOS AND UNITARITY

In a problem involving the decay of a single discrete state $|a\rangle$ into the coupled continua $|ie)$ and $|f\omega)$, $|e\}$ and $|\omega\}$ represent orthogonal free-electron and photon channels into which the state can decay. Each $|e\}$ and $|\omega\}$ is a linear combination of the $|ie)$ and $|f\omega)$ over a range of energies. The diagonalization of the two continua is a unitary transformation, and completeness requires

$$
\begin{aligned}
\langle a|VV|a\rangle &= \int de \langle a|V|e\}\{e|V|a\rangle \\
&\quad + \int d\omega \langle a|V|\omega\}\{\omega|V|a\rangle
\end{aligned}
\tag{9a}
$$

$$
\begin{aligned}
&= \int de\, |\langle a|V|ie)|^2 \\
&\quad + \int d\omega\, |\langle a|V|f\omega)|^2\,.
\end{aligned}
\tag{9b}
$$

However, because the diagonalization mixes states of different energies, in general

$$
\begin{aligned}
&|\langle a|V|e\}|^2+|\langle a|V|\omega\}|^2 \\
&\qquad \neq |\langle a|V|ie)|^2+|\langle a|V|f\omega)|^2\,.
\end{aligned}
\tag{10}
$$

In the PA, in fact, one obtains

$$
\begin{aligned}
&|\langle a|V|e\}|^2+|\langle a|V|\omega\}|^2 \\
&\qquad = \frac{1}{\psi}[\,|\langle a|V|ie)|^2+|\langle a|V|f\omega)|^2]\,,
\end{aligned}
\tag{11}
$$

where ψ can be obtained by making the PA in (5b); one finds

$$\psi=1+\pi^2|H_{e\omega}|^2\,.$$

Since Eq. (11) is just $1/2\pi$ the decay rate of state $|a\rangle$, the continuum-continuum coupling slows the decay of $|a\rangle$ throughout the range of the continua where the PA is valid. Contrary to implications of ATW it is not a measure of unitarity violation: Unitarity is violated only if one integrates (11) over all continuum energies, but this violation simply means that the PA is not valid over the entire continua. Indeed, one can prove explicitly that (9a) equals (9b) by using Eqs. (5) for $|e\}$ and $|\omega\}$ and using the known analytic properties of the self-energies. (The techniques which can be used are illustrated in Sec. IV.)

It is worthwhile to analyze the branching ratios into the continua $|E\}$ and $|\omega\}$ in the PA, as ATW have done. In this approximation all but the lowest order term in ATW's integral equation for the K matrix are identically zero (independent of field strength), and the branching ratios of ATW are identical to those which can be obtained from (5) in the PA on the $\{|ie)\}$ and $\{|f\omega)\}$ continua. One obtains the decay rates and branching ratios

$$\tilde{\Gamma}=\Gamma\frac{1+\gamma^2/\Gamma^2 q_f^2}{\psi^2}\,, \tag{12a}$$

$$\tilde{\gamma}=\gamma\,\frac{1+1/q_f^2}{\psi^2}\,, \tag{12b}$$

where $\Gamma=2\pi|\langle a|V|ie)|^2$, $\gamma=2\pi|\langle a|V|f\omega)|^2$, and where q_f denotes the Fano q value,

$$q_f=\frac{\langle a \mid V \mid f\omega)}{\pi\langle a \mid V \mid ie)H_{e\omega}} . \tag{13}$$

The decay probabilities for the new channels are

$$P_{\rm el}=\frac{\tilde{\Gamma}}{\tilde{\Gamma}+\tilde{\gamma}}=\frac{\Gamma}{\Gamma+\gamma}\frac{1}{\psi}\left[1+\frac{\gamma^2}{\Gamma^2 q_f^2}\right] , \tag{14a}$$

$$P_{\rm ph}=\frac{\tilde{\gamma}}{\Gamma+\tilde{\gamma}}=\frac{\gamma}{\Gamma+\gamma}\frac{1}{\psi}\left[1+\frac{1}{q_f^2}\right] , \tag{14b}$$

where $\psi=1+\pi^2|H_{e\omega}|^2=1+\gamma/q_f^2\Gamma$. Note that the continuum-continuum coupling always acts to enhance the weaker process. These probabilities were first given by ATW, but are more general than they claimed: The only approximation made in their evaluation is the PA on the original continua. No weak-coupling approximations are needed, and these results do not violate unitarity.

IV. UNITARITY VIOLATION IN THE POLE APPROXIMATION

A. General considerations

As mentioned above, unitarity is violated in Eq. (9) if one makes the PA in the self-energies before integrating. Incorrect results can be obtained in other situations as well if one makes the PA before integrating, as Fano showed in his original paper[10] in the context of completeness. One place such difficulties can arise is in performing a sequential diagonalization of discrete state-coupled continua systems. If one first diagonalizes the two continua as above, then in diagonalizing a discrete state $|a\rangle$ into the system one encounters self-energies such as

$$\int de \frac{|\langle a \mid V \mid e\}|^2}{z-e}+\int d\omega \frac{|\langle a \mid V \mid \omega\}|^2}{z-\omega} . \tag{15}$$

These integrals can be evaluated exactly using the analytic properties of the self-energies in the expressions for $|\langle a \mid V \mid e\}|^2$ and $|\langle a \mid V \mid \omega\}|^2$ [Eq. (7)]. One obtains

$$\begin{aligned}\int de \frac{|\langle a \mid V \mid e\}|^2}{E+i\epsilon-e}+\int d\omega \frac{|\langle a \mid V \mid \omega\}|^2}{E+i\epsilon-\omega} &=\Sigma^{aa}(E+i\epsilon)+\frac{1}{\psi(E+i\epsilon)}[\Sigma^{ag}(E+i\epsilon)\Sigma^{fa}(E+i\epsilon)+\Sigma^{af}(E+i\epsilon)\Sigma^{ga}(E+i\epsilon)\\ &\quad+\Sigma^{ag}(E+i\epsilon)\Sigma^{ff}(E+i\epsilon)\Sigma^{ga}(E+i\epsilon)+\Sigma^{af}(E+i\epsilon)\Sigma^{gg}(E+i\epsilon)\Sigma^{fa}(E+i\epsilon)] ,\end{aligned} \tag{16a}$$

where

$$\Sigma^{aa}(E+i\epsilon)=\int de \frac{|\langle a \mid V \mid ie)|^2}{E+i\epsilon-e}+\int d\omega \frac{|\langle a \mid V \mid f\omega|^2}{E+i\epsilon-\omega} . \tag{16b}$$

If one now makes the PA in the self-energies on the right-hand side of (16a), one obtains

$$\int de \frac{|\langle a \mid V \mid e\}|^2}{E+i\epsilon-e}+\int d\omega \frac{|\langle a \mid V \mid \omega\}|^2}{E+i\epsilon-\omega} \approx \frac{-\gamma}{\psi q_f}-\frac{i}{2\psi}(\Gamma+\gamma) . \tag{16c}$$

This result would not have been obtained, however, if the PA were made in the integrands of (16a) before integrating. [The real part of (16c) represents a shift of the decaying state $|a\rangle$, and the imaginary part half its decay rate.]

Thus it is clear that sequential diagonalizations are not always valid if one makes the PA too early. However, there are many situations where such a procedure would be valid and simple. For example, for the two discrete-state continuum system considered by Rzazewski and Eberly[2] the states could be diagonalized into the continuum sequentially using the results of Fano.[10] In the following paragraphs we sketch the criteria one can use to determine if the PA can be made before integrating.

Consider an integral of the form

$$\int dz\, f(z)\Sigma(z) , \tag{17}$$

where $z=E-i\epsilon$ and the path of integration parallels the real axis. The self-energy (SE) $\Sigma(z)$ is analytic (with no poles) on the first Riemann sheet, but has a cut along the positive real axis and poles on the second Riemann sheet. $\Sigma(z)$ can be treated as constant only if $f(z)$ has poles whose residues are much more important than the (second sheet) residues of the poles of $\Sigma(z)$.

Let us suppose a special form for $f(z)\Sigma^{\rm II}(z)$ on the second sheet. [We will denote the second sheet SE by $\Sigma^{\rm II}(z)$.] We take

$$f(z)\Sigma^{\rm II}(z)=\frac{h(z)}{\left[\prod_i(z-p_i)\right]\left[\prod_i(z-q_i)\right]} , \tag{18}$$

where $h(z)$ is entire, p_i are the poles of $f(z)$, and q_i are the poles of the SE. We will assume a "smooth continuum," i.e., that the poles of the SE are all isolated compared to the poles of $f(z)$:

$$|p_i-q_j| \gg |p_i-p_k| \tag{19a}$$

and

$$|q_i-q_j| \gg |p_k-p_l| ,\quad i\neq j \tag{19b}$$

for all i, j, k, and l. The residue at a pole of the potential, say at q_i, is

$$R(q_i)=\frac{h(q_i)}{\left[\prod_j(q_i-p_j)\right]\left[\prod_{j(\neq i)}(q_i-q_j)\right]}\,, \tag{20a}$$

and the residue at a pole p_i of $f(z)$ is

$$R(p_i)=\frac{h(p_i)}{\left[\prod_{j(\neq i)}(p_i-p_j)\right]\left[\prod_j(p_i-q_j)\right]}\,. \tag{20b}$$

It is clear from (19) that

$$|R(q_i)| \ll |R(p_i)| \tag{21}$$

provided there are at least two poles p_i of $f(z)$. [If $f(z)$ has only one pole then we will not have any p_i-p_j terms.] If these poles lie in both half planes, then the poles of the potential can safely be neglected. If $f(z)$ has poles in only one half plane, then the residues at the poles can partially cancel when added together; for this case one could not neglect the poles of the potential, as is clearly shown by the simple fact that one could close the contour in the other half plane. In such a situation, however, the overall integral would be very small.

This suggests that one can neglect the energy dependence of $\Sigma(z)$ in an integral of the form (17) when $f(z)$ has at least two poles, one in each (upper and lower) half plane. If $f(z)$ has two poles, but they lie in the same half plane, then the PA is not valid, but the overall integral will be small.

Examining the integrals (9) and (15) using Eq. (7), we see that the above criteria are not met, and consequently the PA cannot be made before integrating. The matrix elements (7) have no poles themselves other than those in the self-energies or potentials; this is because (7) gives the matrix elements to a diagonalized continuum-continuum system. If we were to consider instead the matrix element to a diagonalized continuum-discrete state system (a Fano continuum), then there would be a pole because of the localization in energy of the original discrete state embedded in the continuum. The matrix element coupling some state $|i\rangle$ to a diagonalized $|a\rangle-\{|E\rangle\}$ (Fano) system $|E_F\rangle$ can be written as

$$\langle i|V|E_F\rangle=\langle i|V|E\rangle+\frac{[\Sigma^{ia}(E-i\epsilon)+\langle i|V|a\rangle]\langle a|V|E\rangle}{E-i\epsilon-E_a-\Sigma^{aa}(E-i\epsilon)}\,, \tag{22a}$$

where

$$\Sigma^{ia}(z)=\int dE\frac{\langle i|V|E\rangle\langle E|V|a\rangle}{z-E}\,, \tag{22b}$$

etc. An integral of the form $\int dE_F\,|\langle i|V|E_F\rangle|^2$ would violate unitarity if the PA were made before integrating, but integrals of the form

$$\int dE_F\frac{|\langle i|V|E_F\rangle|^2}{z-E_F}\,, \tag{23}$$

such as would be encountered in a sequential diagonalization, could be evaluated making the PA before integrating. Consequently, one can sequentially diagonalize discrete states into a continuum, but one cannot make the PA before integrating self-energies in diagonalizing continuum-continuum systems.

B. Specific Example

To illustrate how the analytic properties of the self-energy can be used to evaluate certain integrals, we will consider $\int dE\,|\langle i|V|E_F\rangle|^2$ in detail. The explicit form of the matrix element is given in Eq. (22a). The self-energies $\Sigma^{jk}(E+i\epsilon)$ and $\Sigma^{jk}(E-i\epsilon)$ are analytic[11] in the upper and lower half planes, respectively, but have unknown poles in the opposite half planes. Similarly $[z-E_a-\Sigma^{aa}(z)]^{-1}$ is analytic in the upper or lower half planes for $z=E+i\epsilon$ or $z=E-i\epsilon$. The matrix elements $\langle i|V|E\rangle$ and $\langle a|V|E\rangle$ have poles in both half planes, but their products can be written in terms of the self-energies by

$$\langle j|V|E\rangle\langle E|V|k\rangle=\frac{1}{2\pi i}[\Sigma^{jk}(E-i\epsilon)-\Sigma^{jk}(E+i\epsilon)],\quad j,k=i,a\,. \tag{24}$$

Thus one obtains a fairly messy integral involving self-energies evaluated at both sides of the real axis. One can perform the integral exactly by separating the $\Sigma^{jk}(E+i\epsilon)$ and $\Sigma^{jk}(E-i\epsilon)$ terms. After lengthy algebra one can show that

$$|\langle i|V|E_F\rangle|^2=|\langle i|V|E\rangle|^2+\frac{1}{2\pi i}\frac{[\langle i|V|a\rangle+\Sigma^{ia}(E-i\epsilon)][\langle a|V|i\rangle+\Sigma^{ai}(E-i\epsilon)]}{E-E_a-\Sigma^{aa}(E-i\epsilon)}+\frac{1}{2\pi i}\frac{[\langle i|V|a\rangle+\Sigma^{ia}(E+i\epsilon)][\langle a|V|i\rangle+\Sigma^{ai}(E+i\epsilon)]}{E-E_a-\Sigma^{aa}(E+i\epsilon)}\,. \tag{25}$$

The second and third terms are analytic with no poles in the lower and upper half planes, respectively, and can easily be integrated by closing the contour and subtracting the contribution of the semicircle at infinity. Each integral gives $\frac{1}{2}|\langle i|V|a\rangle|^2$, and therefore

$$\int dE\,|\langle i|V|E_F\rangle|^2=\int de\,|\langle i|V|E\rangle|^2+|\langle i|V|a\rangle|^2\,. \tag{26}$$

V. INTERPRETATION OF THE CONTINUUM-CONTINUUM COUPLING AND THE FANO q VALUE

We conclude this paper with a short discussion of the term "recombination" which ATW use to describe the continuum-continuum coupling and of the Fano q value. We restrict our attention to the problem of a single discrete state $|a\rangle$ decaying into the two coupled continua.

"Recombination" is certainly a physically meaningful term in a scattering problem in which an incoming electron collides with an atom because the continuum-continuum coupling allows the electron to be captured and a photon to be ejected, even in the absence of the discrete state $|a\rangle$. For our problem of interest, however, we do not have an incoming wave packet. We instead start the system in a discrete state at $t=0$ and describe the subsequent decay. The continuum-continuum coupling is important in diagonalizing the total Hamiltonian, but in this context the coupling does *not* imply the physical ejection and subsequent reabsorption of an electron or photon. The actual emission of an electron or photon would still be Markovian (i.e., the emission is effectively instantaneous) for smooth continua. This result is clearly shown by the results of Agarwal, Haan, Burnett, and Cooper[3] who used the method of master equations. They allowed for the continuum-continuum coupling but made the Markov approximation at the outset on the photon continuum. The results obtained in that way agree with the results obtained using resolvents, even though the pole approximation is not made in the latter method until the model problem has been solved exactly.

Our interpretation of the continuum-continuum coupling is simply that what we normally think of as "free-electron" and "free-photon" continua far from the atom are modified near the atom by the coupling of the electron continuum with the bound atomic state $|f\rangle$. Thus, electrons are not physically ejected and then reabsorbed. One must rediagonalize the continua to give the actual "electron" and "photon" continua near the atom.

One can obtain an interesting interpretation of the Fano q value by considering the decay of a discrete state $|a\rangle$ into the continua $\{|ie\rangle\}$ and $\{|f\omega\rangle\}$ in the limits of no direct coupling to one or the other of the original continua. In the limit $\langle a|V|f\omega\rangle\to 0$, the electron and photon emission rates are, respectively,

$$\tilde{\Gamma}_1=\frac{\Gamma}{\psi^2}\,, \tag{27a}$$

$$\tilde{\gamma}_1=\frac{\psi-1}{\psi^2}\Gamma\,. \tag{27b}$$

The photon and electron probabilities are

$$P_{\rm el}=\frac{1}{\psi}\,, \tag{27c}$$

$$P_{\rm ph}=\frac{\psi-1}{\psi}\,. \tag{27d}$$

Thus $\pi^2|H_{e\omega}|^2=1-\psi$ is the probability ratio of the "newly opened" channel to the original channel. A similar analysis can be conducted in the limit $\langle a|V|ie\rangle\to 0$. The results for this case are

$$\tilde{\Gamma}_2=\frac{\psi-1}{\psi^2}\gamma,\quad \tilde{\gamma}_2=\frac{\gamma}{\psi^2},\quad P_{\rm el}=\frac{\psi-1}{\psi},\quad P_{\rm ph}=\frac{1}{\psi}\,. \tag{28}$$

The Fano q value is defined in the PA by Eq. (13). Because the radiative decay is due to the interaction between the atom and the vacuum state of the radiation field for decay from both the discrete state and the electronic continuum, this ratio is equal to the "usual" Fano q value

$$q=\frac{V_{af}}{\pi V_{aE}V_{Ef}}$$

discussed in photoionization and autoionization. The ratio of our two expressions (28) and (27b) for the decay rates into the photon continuum is

$$\frac{\tilde{\gamma}_2}{\tilde{\gamma}_1}=q^2\,, \tag{29}$$

and therefore the square of the Fano q value is the ratio of two rates: The rate for $|a\rangle\to|f\rangle$ transitions in the limit $\langle a|V|ie\rangle\to 0$ divided by the rate for $|a\rangle\to\{|ie\rangle\}\to|f\rangle$ transitions in the limit $\langle a|V|f\omega\rangle\to 0$.

ACKNOWLEDGMENTS

The authors wish to acknowledge helpful conversations with G. S. Agarwal and K. Burnett. This work was supported in part by National Science Foundation Grant No. PHY-82-00805.

[1] L. Armstrong, Jr., C. E. Theodosiou, and M. J. Wall, Phys. Rev. A 18, 2538 (1978).

[2] See, for example, P. Lambropoulos and P. Zoller, Phys. Rev. A 24, 379 (1981); K. Rzazewski and J. H. Eberly, Phys. Rev. Lett. 47, 408 (1981).

[3] G. S. Agarwal, S. L. Haan, K. Burnett, and J. Cooper, Phys. Rev. Lett. 48, 1164 (1982); G. S. Agarwal, S. L. Haan, K. Burnett, and J. Cooper, Phys. Rev. A 26, 2277 (1982); and G. S. Agarwal, S. L. Haan, and J. Cooper, *ibid.* 28, 1154 (1983).

[4] S. L. Haan and G. S. Agarwal, in *Spectral Line Shapes, Proceedings of the Sixth International Conference on Spectral Line Shapes, Boulder, 1982,* edited by K. Burnett (de Gruyter, Berlin, 1983), Vol. 2, p. 1013.

[5] M. Crance and L. Armstrong, Jr., J. Phys. B 15, 3199 (1982).

[6] M. Lewenstein, J. Haus, and K. Rzazewski, Phys. Rev. Lett. 50, 417 (1983).

[7] Explicit forms for $f(e)$ and $g(\omega)$ are given in S. L. Haan, Ph.D. thesis, University of Colorado, 1983 (unpublished).

[8] See, for example, J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972). A minor difficulty arises in the standard scattering theory when quantized fields are involved since the interaction extends too far from the atom. We will not discuss

the elimination of such difficulties or renormalization (see, for example, Ref. 11).

[9]Since the Hamiltonian H^0 already includes some atomic interactions (call them V'), the states $|ie)$ and $|f\omega)$ are not simple plane waves. They could be obtained from plane-wave states by applying the Ω_- corresponding to V', and consequently each $|ie)$, for example, consists of a plane wave plus an incoming spherical wave.

[10]U. Fano, Phys. Rev. 124, 1866 (1961).

[11]M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).