Atomic level shifts and transition amplitudes in incoming radiation fields*

S. Yeh and P. Stehle

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260

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Expressions for energy-level shifts and transition amplitudes of atoms interacting with an incoming radiation field are developed in a completely quantum theoretic way and the results are compared with others. The continued-fraction expressions reproduce both those of Swain and of Gontier et al., and the numerical results for the particular case of Bloch-Siegert shifts in mercury vapor agree with Stenholm's but go further in giving the shape of the resonances. These results are also obtained by a method of direct diagonalization of the Hamiltonian of the coupled system.

I. INTRODUCTION

The effect of a strong incident radiation field on atomic energy levels and on atomic transitions has been much studied. Semiclassical methods were applied first and continue to be used. More recently, purely quantum-mechanical methods have been developed which have, to a large extent, confirmed the predictions of the semiclassical work. Among the semiclassical theories, those of Autler and Townes,[1] of Mollow,[2] and of Stenholm[3] may be mentioned. Quantum theoretic calculations have been done by Cohen-Tannoudji and his co-workers,[4,5] by Chang and Stehle,[6] by Swain,[7] by Gontier and co-workers,[8] and by Bialynicki-Birula and Bialynicka-Birula,[9] among others. While it is obvious in principle that semiclassical and fully quantum theories are distinct, it is by no means so clear under what conditions they will give different results. The results we achieve in this paper do not demonstrate any such difference. What we do accomplish is to derive easily used expressions for Green's functions (resolvents) and transition amplitudes for multilevel atoms interacting with intense incoming radiation described in a completely quantum theoretic way. We are able to give a unified and direct derivation of continued-fraction expressions appearing in the work of Gontier, Rahman, and Trahin,[8] and of Swain.[7] In addition a straightforward method based on the diagonalization of a truncated Hamiltonian describing an atom coupled to a single field mode is given. The theory is applied to experiments of Arimondo and Moruzzi,[10] who measured Bloch-Siegert shifts in mercury vapor.

The advantage of continued-fraction expressions is the automatic inclusion of all proper diagrams up to the order in perturbation theory desired in an extremely simple way. The advantage of the derivation given here is its relative simplicity and its independence of a model such as a two-level atom or a single mode field. The derivation is based on the "level shift" operator used by Goldberger and Watson,[11] and is a straightforward exercise in quantum mechanics. It is equivalent to the forward scattering method of Chang and Stehle,[6] yielding expressions of the same form as theirs, but developing them further.

A convenient way of describing atom-field interactions by means of walk diagrams is introduced. The use of such diagrams, closely related to Feynman diagrams, makes the counting of processes easy and serves to clarify the various continued fractions and other interaction schemes that are available.

II. HAMILTONIAN

The system of concern is an atom interacting with a field. For the general discussion in Sec. III we need not specify the system more closely than to say there is a Hamiltonian H_0 describing the atom and field in the absence of coupling, and a coupling $V = V_+ + V_-$, which acts to cause the absorption or emission of field quanta one at a time. In Sec. IV more specific assumptions will be made. Only one field mode will be considered, and only two atomic levels. It will also be assumed that V changes the atomic state, as required by electric dipole selection rules for example, but the rotating-wave approximation will not be made. For intense field problems it is also permissible to neglect depletion effects, which means only that the coupling constant measuring the atom-field interaction can be considered a constant independent of the number of quanta which have been emitted or absorbed. This approximation is not essential, and depletion can be taken into account if desired. The coupling is characterized by

$$\xi = (e^2 N \omega / 2V)^{1/2} \langle a|\hat{d}|b\rangle, \qquad (2.1)$$

where N/V is the photon density, ω is the field frequency, and $\langle a|\hat{d}|b\rangle$ is the relevant dipole matrix element, taken to be real. Mode indices may be

added to N, ω, and the matrix element, if more than one is considered.

III. GREEN'S FUNCTION FORMULATION

The time development of the system atom-plus-field is described by the Green's function $G(t_2, t_1)$. When the Hamiltonian is time independent, this is a function of $t_2 - t_1$, while if the field is a specified classical field, as in the semiclassical theory, the time arguments appear separately and an average must be found over the phase of the field at the earlier time, as this is not experimentally controlled. We consider here the time-independent Hamiltonian including the field degrees of freedom. Then we may write

$$G(t_2 - t_1) = \frac{1}{2\pi i} \int dE\, G(E) \exp[-iE(t_2 - t_1)], \quad (3.1)$$

and study the Green's function $G(E)$. The poles of $G(E)$ define the energy eigenvalues of the coupled system in the standard way.

If H is the complete Hamiltonian and H_0 is the Hamiltonian of the uncoupled atom and field, then

$$G(E) = \frac{1}{E - H}, \quad G_0(E) = \frac{1}{E - H_0}. \quad (3.2)$$

$G(E)$ satisfies the integral equation

$$G(E) = G_0(E) + G_0(E) V G(E). \quad (3.3)$$

We introduce projection operators P_N, which project onto the space of states containing N photons, independent of the atomic state:

$$P_N^2 = P_N, \quad [P_N, H_0] = 0. \quad (3.4)$$

We shall call

$$G_N(E) = P_N G(E) P_N \quad (3.5)$$

a diagonal Green's function. It is an operator in the space of N-photon states and the atomic states. The Green's function

$$G(E) P_N = F(E) G_N(E) \quad (3.6)$$

has matrix elements connecting N-photon states with all other states. Following a method of Goldberger and Watson,[11] we find an expression for $F(E) P_N$.

$G(E)$ satisfies the equation

$$(E - H_0) G = 1 + VG, \quad (3.7)$$

so that

$$(E - H_0) F G_N = P_N + V F G_N. \quad (3.8)$$

From this,

$$G_N = \frac{P_N}{E - H_0 - P_N V F P_N}, \quad (3.9)$$

because

$$P_N F P_N = P_N. \quad (3.10)$$

Now rewrite (3.8) as

$$(E - H_0 - \Theta) F G_N = P_N + (V - \Theta) F G_N, \quad (3.11)$$

where Θ is to be determined later. This can be written as

$$FP_N = \frac{1}{E - H_0 - \Theta} P_N [E - H_0 - P_N V F P_N]$$

$$+ \frac{1}{E - H_0 - \Theta} (V - \Theta) F P_N. \quad (3.12)$$

On choosing

$$\Theta = P_N V F P_N, \quad (3.13)$$

this simplifies to

$$FP_N = P_N + \frac{1}{E - H_0 - P_N V F P_N} (V - P_N V F P_N) F P_N$$

$$= P_N + \frac{1}{E - H_0 - P_N V F P_N} (1 - P_N) V F P_N$$

$$= P_N + \frac{1 - P_N}{E - H_0} V F P_N. \quad (3.14)$$

The second step is a consequence of (3.10), and the third step of a geometric series expansion in which each term after the first contains the factor $P_N(1 - P_N) = 0$. Equation (3.14) can be iterated to give another geometric series which can be summed

$$FP_N = P_N + \frac{1 - P_N}{E - H_0} V P_N + \frac{1 - P_N}{E - H_0} V \frac{1 - P_N}{E - H_0} V P_N + \cdots$$

$$= P_N + \frac{1}{E - H_0 - V_N} V P_N, \quad (3.15)$$

with

$$V_N = (1 - P_N) V (1 - P_N). \quad (3.16)$$

V_N has no nonzero matrix elements connecting N-photon states with others. From (3.15) we obtain

$$P_N V F P_N \equiv \Theta = P_N V \frac{1}{E - H_0 - V_N} V P_N, \quad (3.17)$$

and consequently

$$G_N(E) = \frac{P_N}{E - H_0 - P_N V[1/(E - H_0 - V_N)] V P_N}, \quad (3.18)$$

where we have used the property of V that

$$P_N V P_M \neq 0 \text{ implies } M = N \pm 1$$

to omit the term $P_N V P_N$. We insert $\sum_M P_M = 1$ between V and $(E - H_0 - V_N)^{-1}$ in the denominator of (3.18), and $\sum_{M'} P_{M'} = 1$ between $(E - H_0 - V_N)^{-1}$ and

V. In each case only $M = N \pm 1$ or $M' = N \pm 1$ contributes. Terms containing

$$P_{N \pm 1} \frac{1}{E - H_0 - V_N} P_{N \mp 1}$$

$$G_N(E) = \frac{P_N}{E - H_0 - P_N V P_{N+1}(E - H_0 - V_N)^{-1}P_{N+1}VP_N - P_N VP_{N-1}(E - H_0 - V_N)^{-1}P_{N-1}VP_N}$$

$$\equiv \frac{P_N}{E - H_0 - P_N VG_{N+1}(E, V_N)VP_N - P_N VG_{N-1}(E, V_N)VP_N}, \tag{3.19}$$

where $G_{N \pm 1}(E, V_N)$ is a diagonal Green's function between $N \pm 1$ photon states formed with V_N as the interaction instead of V.

Equation (3.19) is not itself solvable by iteration because the left side is not of the proper form to substitute into the denominator of the right side. Now, however, we may write the analog of (3.19) for the diagonal Green's function $G_{N+1}(E, V_N)$ simply by replacing N by $N+1$ and V by V_N in (3.19). On doing this to the last term in the denominator, we get

$$P_{N+1}V_N G_N(E, V_{N+1})V_N P_{N+1} = 0,$$

because

$$V_N G_N = (1 - P_N)V(1 - P_N)P_N GP_N = 0;$$

so the equation for $G_{N+1}(E, V_N)$ is simply

$$G_{N+1}(E, V_N) = \frac{P_{N+1}}{E - H_0 - P_{N+1}V_N G_{N+2}(E, V_{N+1})V_N P_{N+1}}$$

$$= \frac{P_{N+1}}{E - H_0 - P_{N+1}VG_{N+2}(E, V_{N+1})VP_{N+1}} \tag{3.20}$$

This can be developed into a continued fraction by iteration, and the same can be done for $G_{N-1}(E, V_N)$. Finally, $G_N(E)$ is given by an expression involving two continued fractions in the denominator, similar in structure but simpler than the expression of Gontier et al., which we derive below.

The structure of $G_N(E)$ and of $G_{N \pm 1}(E, V_N)$ is easily visualized in terms of walks.[12] $G_N(E)$ is represented by a walk whose steps to the right toward larger N are caused by V_-, and whose steps to the left, toward smaller N, by V_+. In a given order of perturbation theory, a specific number of steps is involved; in general there may be any number from none to infinity, but there must be equal numbers to right and to left for diagonal Green's function. Figure 1 illustrates (3.19) and (3.20). What appear in these figures are proper walks which start from N and do not return there

do not contribute, because V_N has no matrix element connecting with an N-photon state, and so no product of V_N's can connect an $N+1$ photon state with an $N-1$ photon state. The diagonal Green's function now take the form

until the last step. In Fig. 1(a) one walk starts to the right and one to the left. There is also a walk with no steps. These appear in the denominator of the Green's function, and in a geometric series expansion they then appear in all possible sequences, including repetitions. $G_{N+1}(E, V_N)$ is represented by walks remaining to the right of N, as they cannot ever reach N by action of V_N. Similarly, the walks representing $G_{N-1}(E, V_N)$ remain to the left of N.

The form of $G_N(E)$ given by Gontier et al. is obtained from (3.18) by iterating the Green's function in the denominator twice, using the appropriate
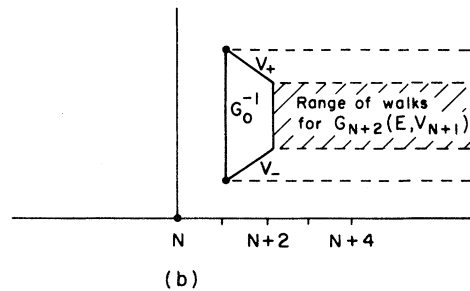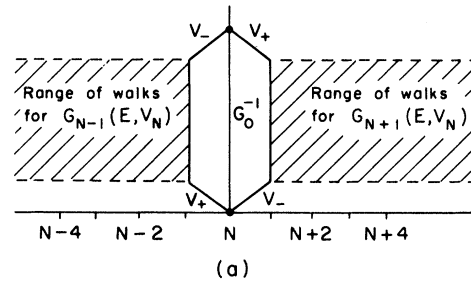

FIG. 1. (a) Proper walks from N to N consist of a direct passage with no sidestep, and of arbitrary walks staying on or to the right of $N+1$, and on or to the left of $N-1$. (b) Walks representing $G_{N+1}(E, V_N)$ must stay to the right of $N+1$, because V_N connects N with nothing.

order of factors

$$\frac{1}{E-H_0-V_N} = \frac{1}{E-H_0} + \frac{1}{E-H_0}\,V_N\left(\frac{1}{E-H_0} + \frac{1}{E-H_0-V_N}\,V_N\frac{1}{E-H_0}\right) = G_0 + G_0 V_N G_0 + G_0 V_N\frac{1}{E-H_0-V_N}\,V_N G_0.$$

$$(3.21)$$

Using this, (3.18) becomes

$$G_N(E) = \frac{P_N}{E-H_0-P_N VG_0 VP_N - P_N VG_0 V_N(E-H_0-V_N)^{-1}V_N G_0 VP_N}$$

$$(3.22)$$

Arguments like those used in deriving (3.19) from (3.18) enable us to write this as

$$G_N(E) = P_N\left(E-H_0-P_N W_0 P_N - P_N W_+ P_{N+2}\frac{1}{E-H_0-V_N}P_{N+2}W_-P_N - P_N W_-P_{N-2}\frac{1}{E-H_0-V_N}P_{N-2}W_+P_N\right)^{-1}$$

$$= P_N[E-H_0-P_N W_0 P_N - P_N W_+ G_{N+2}(E,V_N)W_-P_N - P_N W_- G_{N-2}(E,V_N)W_+P_N]^{-1},$$

$$(3.23)$$

where

$$W_0 = V_+ G_0 V_- + V_- G_0 V_+,$$

$$W_+ = V_+ G_0 V_+, \quad W_- = V_- G_0 V_-,$$

$$(3.24)$$

and $V_\pm$ are the positive frequency (absorption) and negative frequency (emission) parts of V.

The diagonal Green's function $G_{N+2}(E,V_N)$ can be expanded in powers of V_N, and because V changes

the photon number by unity, all odd powers of V_N drop out. The resulting series can then be re-summed to give

$$G_{N+2}(E,V_N) = P_{N+2}\frac{1}{E-H_0-V_N G_0 V_N}P_{N+2}.$$

$$(3.25)$$

Again, we may write the analog of (3.23) for $G_{N+2}(E,V_N G_0 V_N)$, and obtain a form suitable for iteration into a continued fraction:

$$G_{N+2}(E,V_N G_0 V_N) = \frac{P_{N+2}}{E-H_0-P_{N+2}W_0 P_{N+2} - P_{N+2}W_+ G_{N+4}(E,V_N G_0 V_N)W_-P_{N+2}}$$

$$(3.26)$$

A similar continued-fraction expansion of $G_{N-2}(E,V_N G_0 V_N)$ also exists.

The connection with the expressions of Gontier et al. is established by introducing the notations

$$T = G_0 W_0, \quad X = G_0 W_+, \quad Y = G_0 W_-$$

$$\mathcal{T}_\square G_0 = G_N(E),$$

$$(3.27)$$

$$\mathcal{T}^{(1)}G_0 = G_{N-2}(E,V_N), \quad \mathcal{T}^{(2)}G_0 = G_{N+2}(E,V_N).$$

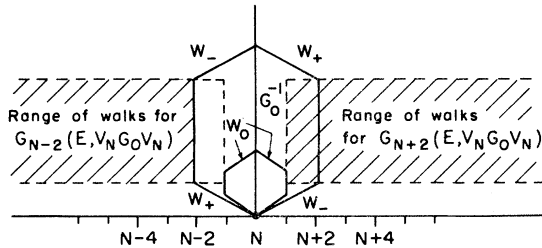The walk representation of (3.23) is shown in Fig.

FIG. 2. In the denominator of $G_N(E)$ there appear G_0^{-1} represented by the vertical line; W_0 represented by the simplest possible walks, and the general walks in the indicated ranges. The vertical scale, measuring the number of steps, is defined only in each order of perturbation theory.

2. All sequences of the walks represented occur in the full Green's function.

The relation of walks to Feynman diagrams is simple; a photon emission is a step to the right, a photon absorption a step to the left. The advantage of walks over Feynman diagrams is simply the direct representation of the total number of photons in the field at each stage. Using walks it is easy to count the total number of forward scattering diagrams, and of proper forward scattering diagrams in any order of perturbation theory.

Off-diagonal elements of $G(E)$ can also be obtained. If $N' > N$, from (3.6) and (3.15) we obtain

$$P_{N'}GP_N = P_{N'}FG_N = P_{N'}\frac{1-P_N}{E-H_0-V_N}VG_N$$

$$= P_{N'}\frac{1}{E-H_0-V_N}P_{N+1}V_- G_N$$

$$= P_{N'}G(E,V_N)P_{N+1}V_- G_N.$$

$$(3.28)$$

The degree of being off diagonal is reduced by one, and the process can be repeated as often as needed. If $N' = N+1$, (3.28) is sufficient as

$$P_{N+1}GP_N = P_{N+1}G(E,V_N)P_{N+1}V_- G_N(E),$$

$$(3.29)$$

and only diagonal elements are involved. This equation can be read as follows: The system propagates from the initial N-photon state to N-photon states which it then leaves never to return, and propagates via $G(E, V_N)$ to the $N+1$ photon states. This description can easily be extended to $N' > N+1$. Equation (3.28) is illustrated in Fig. 3.

If the interaction V contains coupling to only a single field mode, the diagonal Green's function describes the forward scattering of photons in this mode, and the operator $\Theta = P_N V[E - H_0 - V_N]^{-1} V P_N$ is the atomic self-energy arising from forward scattering. This approach to the problem of level shifts in incident fields was introduced by Chang and Stehle.[6] In applying the method to two-level atoms, all diagrams automatically included in the continued-fraction expressions were not included by them, so that certain significant diagrams were omitted in their evaluation of Bloch-Siegert shifts. These omissions are corrected in the calculations described in Sec. IV.

Recently Bialynicki-Birula and Bialynicka-Birula[13] have described an "improved iteration procedure" for the evaluation of both diagonal and off-diagonal Green's functions for two-level atoms interacting with a single field mode. Each iteration increases the range of walks included almost in geometrical progression rather than in arithmetic progression, as with the continued fractions developed here, but as a consequence each step is more complicated. It is not clear that there is great advantage of either over the other for computational purpose. The grouping of walks in their procedure is illustrated in Fig. 4.

IV. APPLICATION TO THE SINGLE-MODE TWO-LEVEL PROBLEM

While the projection-operator formalism described in Sec. III applies to the general case of many levels and many modes, it is of interest to demonstrate the application to two-level single-mode problems. In this case, as we will see, the matrix elements, both diagonal and off-diagonal, of the Green's-function operator $G(E)$ have par-
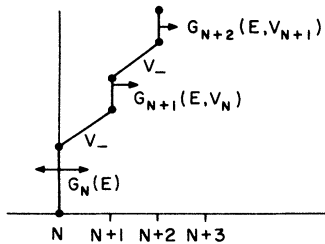
FIG. 3. Walks representing $P_{N'} G(E) P_N$ for $N' = N+2$. They are confined to successively more restricted areas.
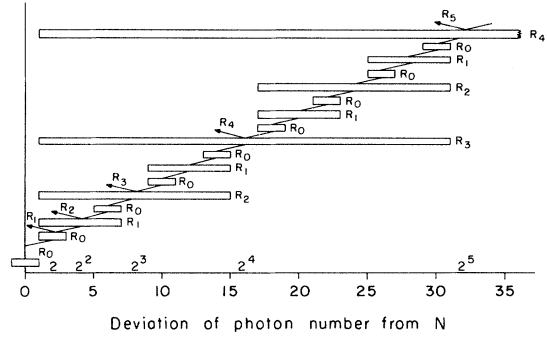
FIG. 4. The improved iteration procedure of the Bialynicki-Birula and Bialynicka-Birula groups walks into the simplest walk R_0, and sequences of walks as shown. The boxes represent complete sets of walks within the limits of the box, not just proper walks relative to the center of the box. Only the steps to the right in each iteration are shown; an identical set of steps to the left returning to the y axis is indicated by the arrows. The reflection of this entire diagram in the y axis must also be included. All walks represented are proper relative to the y axis.

ticularly simple forms.

From Eq. (3.1), the transition amplitude for the system to go from an initial state $|i\rangle$ at time $t = 0$ to a final state $|f\rangle$ at time t is

$$C_{i \to f}(t) = \frac{1}{2\pi i} \int dE \langle f | G(E) | i \rangle e^{-iEt}, \qquad (4.1)$$

and the probability

$$P_{i \to f}(t) = |C_{i \to f}(t)|^2. \qquad (4.2)$$

The matrix element

$$\langle f | G(E) | i \rangle = \langle f | P_f G(E) P_i | i \rangle, \qquad (4.3)$$

if we take $P_f = |f\rangle\langle f|$, $P_i = |i\rangle\langle i|$ being the projection operators onto the subspace $\{|i\rangle\}$ and $\{|f\rangle\}$, respectively. We will use Eqs. (3.19), (3.20), and (3.28) to calculate this matrix element.

Let $|a\rangle$ and $|b\rangle$ be the two states of the atom with energies E_a and E_b in the absence of the field, $E_b - E_a = \omega_0$. Let $|\alpha, N\rangle$ be the state of the system of atom plus field when the atom is in state $|\alpha\rangle$ and the field is in a number state $|N\rangle$, $\alpha = a, b$.

In the Hamiltonian, we have assumed the interaction between the atom and the field is such that every emission and absorption of a photon is accompanied by a change of atomic state. This means, in the case of two-level atom, if we start the system in the state $|a, N\rangle$, it never ends in state $|a, N+m\rangle$ with odd m or $|b, N+m\rangle$ with even m, i.e., the possible final states are

$$|a, N+m\rangle, \quad m \text{ even},$$

and

$|b, N+m\rangle$, m odd,

where m can be positive or negative. Hence we consider the matrix elements

$\langle a, N+m | G(E) | a, N\rangle$, m even,

$\langle b, N+m | G(E) | a, N\rangle$, m odd.

Also, the projection operators P_{N+m} is a pro-

jection operator onto a one-state subspace, i.e.,

$$P_{N+m} = \begin{cases} |a, N+m\rangle\langle a, N+m|, & m \text{ even,} \\ |b, N+m\rangle\langle b, N+m|, & m \text{ odd.} \end{cases}$$

Under these circumstances the diagonal Green's function is not an operator in a multidimensional state space, but is just a matrix element, and (3.19) becomes

$$\langle a, N | G(E) | a, N\rangle = \cfrac{1}{E - E_a - N\omega - \cfrac{\xi^2}{E - E_b - (N-1)\omega - \cfrac{\xi^2}{E - E_a - (N-2)\omega - \xi^2 \atop \ddots}} - \cfrac{\xi^2}{E - E_b - (N+1)\omega - \cfrac{\xi^2}{E - E_a - (N+2)\omega - \xi^2 \atop \ddots}}}$$

$$(4.4)$$

where

$$\xi = (e^2 N\omega / 2V)^{1/2} \langle a | \hat{d} | b\rangle \qquad (4.5)$$

and ω is the photon energy.

In getting Eq. (4.4), we have neglected the depletion of the photons, but it is not essential since we can vary the number of photons N in ξ at every stage. Apart from this, (4.4) is éxactly the same as that obtained by Swain,[14] but the use of projection operators here has greatly simplified the deriva-

$$\langle N+m, \alpha | G(E) | N, a\rangle = \begin{cases} \langle N, a | G(E) | N, a\rangle \xi^m \mathfrak{D}_1 \mathfrak{D}_2 \cdots \mathfrak{D}_m, & \text{positive } m \\ \langle N, a | G(E) | N, a\rangle \xi^{|m|} \mathfrak{D}_{-1} \mathfrak{D}_{-2} \cdots \mathfrak{D}_{-m}, & \text{negative } m, \end{cases} \qquad (4.6)$$

where $\alpha = a$, when m is even, $\alpha = b$ when m is odd, and

$$\mathfrak{D}_m = \begin{cases} \cfrac{1}{E - b_m - \cfrac{\xi^2}{E - b_{m+1} - \xi^2 \atop \ddots}}, & \text{positive } m, \\[4ex] \cfrac{1}{E - b_m - \cfrac{\xi^2}{E - b_{m-1} - \xi^2 \atop \ddots}}, & \text{negative } m, \end{cases} \qquad (4.7)$$

with

$$b_m = \begin{cases} E_b + (N+m)\omega, & m \text{ odd,} \\ E_a + (N+m)\omega, & m \text{ even.} \end{cases}$$

Equations (4.6) can also be obtained by taking the matrix elements of Eq. (3.3) between states with photon numbers differing by one, and solving the set of infinite simultaneous algebraic equations as pointed out by Bialynicka-Birula.[13]

Now that we have the digaonal and off-diagonal matrix elements of $G(E)$, it is not difficult to evaluate the integral in (4.1) using the calculus of residues.

tion. In the language of forward scattering of Chang and Stehle,[6] the two continued fractions in the denominator of (4.4) are just the matrix elements of the forward scattering mass operator. The first one corresponds to the forward scattering process in which the first vertex is an absorption and the second corresponds to those with the first vertex an emission.

For the off-diagonal matrix element, we use P_{N+m} for $P_{N'}$ in (3.28) and follow the same procedure as in the diagonal case. We have

If

$$\langle N+m, \alpha | G(E) | N, a\rangle = 1/f_m(E), \qquad (4.8)$$

the energy eigenvalues E_λ are the zeros of $f_m(E)$, and

$$\frac{1}{2\pi i} \int dE \langle N+m, \alpha | G(E) | N, a\rangle e^{-iEt} = \sum_\lambda \frac{e^{-iE_\lambda t}}{f'_m(E_\lambda)}. \qquad (4.9)$$

This can be easily evaluated numerically.

In the diagonal matrix element, if the continued fractions are truncated at some stage, the resulting finite ones can be expressed as ratios of two polynomials, It is known that the zeros of the denominator are all real and the residues are all positive and have unit sum.[15,16] Poles of the matrix elements correspond to the stationary states of the total Hamiltonian, including both atom and field; so the number of poles included is the number of states of the system that are considered to be superposed in any given truncation. If only two poles are included, one gets the usual Rabi for-

mula. This can be described as the next-to-lowest
order Weisskopf-Wigner approximation in the
sense of Grimm and Ernst,[17] the lowest order being
the rotating-wave approximation with no Bloch-
Siegert shifts. When more poles are included,
states of the system involving photon numbers dif-
fering more from the initial one are included, cor-
responding to the higher-order Weisskopf-Wigner
approximation. This interpretation is closely re-
lated to the level-crossing and anticrossing dia-
grams of Cohen-Tannoudji et al.[4,5]

In the off-diagonal matrix elements (4.6), the
additional continued fractions $\mathfrak{D}_m$'s do not introduce
extra poles. If the $\mathfrak{D}_m$'s are written as the ratio of
the two polynomials, the denominator of $\mathfrak{D}_m$ is ex-
actly the numerator of $\mathfrak{D}_{m-1}$ for positive m, so
that the zeros of the denominator of $\mathfrak{D}_m$'s do not
lead to poles. The same thing can be said for neg-
ative m.

In the experiment of Arimondo and Moruzzi,[10]
the measurement of the Bloch-Siegert shift in op-
tically oriented [189]Hg vapor was done for single-
photon and three-photon transitions. For this ex-
periment, it is enough to calculate the time-aver-
aged transition probability, but we also have to
sum over all possible final photon number states
because the final photon number is not observed.
So, what we really want to calculate is

$$P_{a\to b} = \sum_{m \text{ odd}} \left\langle \left| \frac{1}{2\pi i} \int dE \langle N+m, b|G(E)|N,a\rangle e^{-iEt} \right|^2 \right\rangle_t,$$

(4.10)

where $\langle \cdots \rangle_t$ means the time average and the sum-
mation runs over odd m only.

$P_{a\to b}$ is a function of three parameters ω_0, ω,
and ξ. In the experiment of interest, the RF pho-
ton energy ω is kept constant, the atomic level
separation ω_0 is varied by changing the Zeeman
static magnetic field. For different RF field in-
tensities, i.e., different ξ, the resonant ω_0 is de-
termined as that maximizing $P_{a\to b}$. We follow the
same procedure here to determine the resonant
positions. Typical resonant curves for two RF in-
tensities are plotted in Fig. 5 to show the shifted
resonant positions and power-broadened peaks for
one- and three-photon resonances. The resulting
Bloch-Siegert shifts as a function of RF intensity
are plotted in Fig. 6. Notice that the locations at
which the resonant $\omega_0 = 0$ are $\xi = 1.2024$ for one-
photon case and $\xi = 2.7600$ for three-photon case,
in agreement with the exact solution, these ξ's
being proportional to the first two zeros of the
Bessel's function of order 0.

During the course of numerical evaluation, the
number of poles to be taken, i.e., the stage of
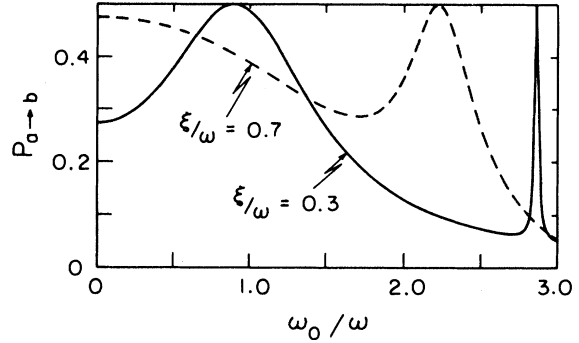truncation of the continued fractions, is determined

FIG. 5. Time-averaged transition probability. Both
one-photon and three-photon resonances are shifted and
broadened as ξ increases. For $\xi/\omega = 0.7$, the one-photon
resonant ω_0 has passed $\omega_0 = 0$.

by increasing the number of poles until the transi-
tion probability is stabilized.

In (4.4), if we truncate the first continued frac-
tion at the first stage and neglect the second one
altogether, we have the rotating-wave approxima-
tion and only the proper walk (a) in Fig. 7 and its
iterations are included in the forward scattering
mass operator or level shift. The first stage of
the second continued fraction contributes the prop-
er walk (b) of Fig. 7 and corresponds to the lowest-
order counter-rotating wave. Including both first
stages thus includes all walks between $N \pm 1$ in the
Green's function. Going to the second state in both
continued fractions includes the proper walks (c)
of Fig. 5, and the Green's function then includes
all walks between $N \pm 2$. The general case is now
clear. The further one goes before truncation, the
wider the range of included walks. The range of
included walks is a more convenient characteriza-
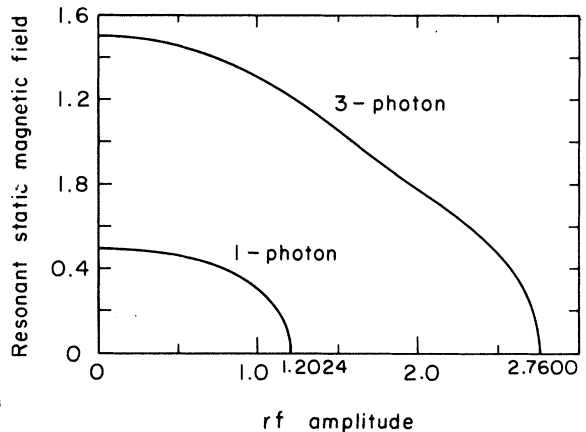tion of the degree of approximation than the num-

FIG. 6. Bloch-Siegert shifts. The scale is the same as
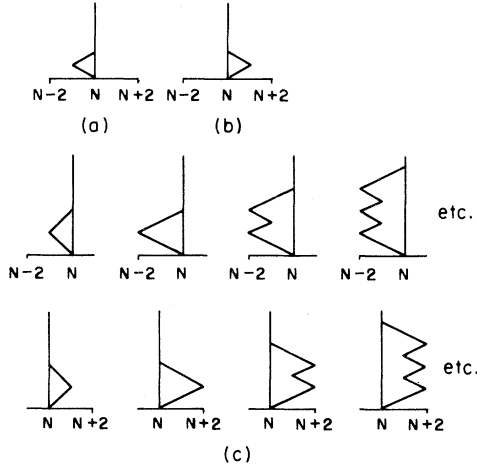that in Ref. 10.

FIG. 7. Walk (a) and its iterations yield the rotating-wave approximation for a two-level atom interacting with a single-mode field. Adding walk (b) includes the counter-rotating wave, and yields the lowest-order Bloch-Siegert shift. The proper walks (c) are those included, together with all their combinations, in the truncation of (4.4) at the second stage.
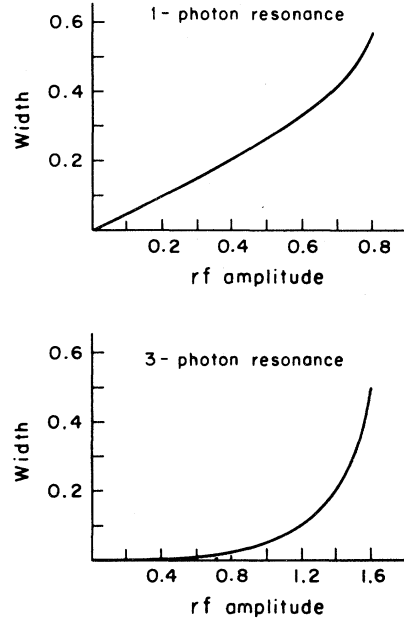

FIG. 8. Widths at 80% peak height. The scale is the same as in Fig. 6. (a) One-photon resonance, the plot is limited to $\xi \le 0.8$ due to the overlap with three-photon resonance. (b) Three-photon resonance for $\xi \le 1.6$ due to the same reason as Fig. 8(a).

ber of steps, which is the same as the order in perturbation theory.

Using the present approach, the widths of the one-photon and three-photon resonances can also be predicted. Looking at Fig. 5, we see that due to power broadening, the two resonance peaks are overlapping for higher RF intensities. It is not possible to determine the full width at half height. Instead, we plot the full width at 80% peak height, to see how the resonance is power broadened. The results are shown in Fig. 8. For lower intensities the width of the one-photon resonance is linear in ξ, and of the three-photon resonance is proportional to ξ^3.

While the projection-operator technique is used in the resolvent formalism of Cohen-Tannoudji,[4,5] it is essentially a perturbation expansion in the mass operator, which in a sense is different from the conventional perturbation expansion. But we have shown here that the repeated uses of the same operator technique lead to the continued-fraction expression for the mass operator, and it converges much faster in the sense that if we truncate at one stage further, infinitely many more diagrams are included as discussed above. Also, they evaluated the resonance position using a two-pole approximation together with the condition $\partial E/\partial \omega_0 = 0$. The accuracy of the two-pole approximation is difficult to estimate when the intensity is high.

We end this section by noting that the Bloch-Siegert shifts obtained above are in exact numerical agreement with those of Stenholm.[3] However,

in the context of Stenholm's semiclassical theory, the Hamiltonian is time-dependent, and consequently there are no energy eigenstates. The physical interpretation of the poles, especially when more than two occur, is obscure. We have also obtained the shape of the resonances with no adjustable parameters, such as Stenholm's phenomenological pumping and damping parameters.

V. DIAGONALIZATION OF THE TOTAL HAMILTONIAN

The transition probability considered in Sec. IV can also be calculated by diagonalizing the total Hamiltonian. The state of the system at time t is

$$|t\rangle = e^{-iHt}|i\rangle, \tag{5.1}$$

by applying the time evolution operator to the state $|i\rangle$ at time $t = 0$. The transition amplitude to a state $|f\rangle$ at the general time t is then

$$C_{i \to f}(t) = \sum_\lambda \langle f|E_\lambda\rangle\langle E_\lambda|i\rangle e^{-iE_\lambda t}, \tag{5.2}$$

where $|E_\lambda\rangle$ is the eigenvector of H with eigenvalue E_λ.

For the two-level single-mode problem, the time-averaged transition probability is

$$P_{a \to b} = \sum_{\substack{k \text{ odd} \\ \lambda}} |\langle b, N+k|E_\lambda\rangle\langle E_\lambda|a, N\rangle|^2. \tag{5.3}$$

The Hamiltonian being considered couples state $|a, N\rangle$ with states $|b, N\pm 1\rangle$ only. Therefore there is no direct or indirect coupling of $|a, N\rangle$ with $|a, N+m\rangle$ when m is odd, or with $|b, N +m\rangle$ when m is even, and then two sets of states can be treated separately. Within one of these sets the Hamiltonian matrix has a tridiagonal form

$$
(H) = \begin{array}{c} \\ |a, N-2\rangle \\ |b, N-1\rangle \\ |a, N\rangle \\ |b, N+1\rangle \\ |a, N+2\rangle \\ \\ \end{array}
\begin{array}{c}
\cdots |a, N-2\rangle \quad |b, N-1\rangle \quad |a, N\rangle \quad |b, N+1\rangle \quad |a, N+2\rangle \cdots \\
\left[
\begin{array}{ccccc}
E_a + (N-2)\omega & \xi & & & \\
\xi & E_b + (N-1)\omega & \xi & & \\
& \xi & E_a + N\omega & \xi & \\
& & \xi & E_b + (N+1)\omega & \xi \\
& & & \xi & E_a + (N+2)\omega
\end{array}
\right]
\end{array}
$$

To study the time development of a state containing N photons, initially one selects a finite segment of this infinite matrix containing the initial state and those within a certain range of photon numbers around it, diagonalizes it, and applies (5.3) with the summation restricted to the selected range. The selection of the range of states to be included is equivalent to choosing the stage of truncation of the continued fractions of Sec. IV, and it determines the maximum excursion of the included walks from the initial photon number. The actual calculation is done numerically, the range of states being increased until the results are stable within the desired accuracy.

This method can be extended to more than two atomic levels in a straightforward way; the resulting Hamiltonian matrix has a band of nonzero elements along the diagonal. Here also, the states separate into two independent sets if the atomic states are like Zeeman states with coupling only between adjacent ones. In this way the experiments of Arimondo and Corbalan[18] on ^{87}Rb, and of Kusch[19] on ^{39}K can be analyzed. As applied to the two-level system of Arimondo and Moruzzi, the diagonalization method yields exactly the same results as obtained in Sec. IV.

VI. CONCLUSIONS

The theoretical analysis of the interaction of an atom with an incoming radiation field given here provides a clear physical picture of the fundamental processes involved and of the meaning of the iteration procedure used in numerical evaluation of the physical quantities desired, the transition probabilities and the shapes of resonances. In the case of a single field mode, the effects of the incoming field are most naturally described in terms of forward scattering, as has been appreciated in treatments of scattering by free electrons for a long time. This interpretation provides the clearest connection with the standard quantum electrodynamic treatments of level shifts arising from vacuum fields. The derivation of the diagonal and off-diagonal Green's function does not, however, involve any of the complications associated with the treatment of virtual photons.

We have provided a unified derivation of results already given by Swain[7] and by Gontier et al.[8] and in the direct diagonalization method we have given an equivalent way of preceeding which is simpler to apply to the problem of many level atoms. The Green's-function approach in this case involves the complication that the effective interaction V_N occurring in the continued fraction is an operator in the space of atomic states, a fact which introduces formidable technical complications in numerical calculations.

The walk diagrams we have introduced furnish a means of specifying the order of approximation used in numerical calculation, and provide a clear picture of the structure of both the diagonal and off-diagonal Green's functions. The advantage over the usual Feynman diagrams is that the order of approximation, which is distinct from an order of perturbation theory, is made manifest.

We do not fully understand the relation of this work to that of Stenholm.[3] The results for the Bloch-Siegert shifts are identical with his, but Stenholm's theory includes in an essential way a pumping and a damping parameter whose values do not affect the position of the resonance but seem to affect its shape. No such parameters occur here.

ACKNOWLEDGMENTS

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