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Continued fraction expressions for the eigensolutions of the hamiltonian describing the interaction between a single atom and a single field mode: comparisons with the rotating wave solutions

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Abstract. Formally exact continued fraction expressions for the eigenvectors and eigenvalues of the hamiltonian describing the interaction of a single atom with a single quantized field mode in the electric dipole approximation are presented. Explicit expressions for the eigensolutions and the time dependent properties are given in some special cases. Comparisons are made with the corresponding rotating wave solutions.

1. Introduction

In a previous publication (Swain 1973, to be referred to as I) we have obtained exact continued fraction expressions describing the time dependent behaviour of a single, two-level 'atom' interacting with a single quantized field mode in the dipole approximation without having recourse to the rotating wave approximation (RWA). In order to complete the formal discussion of this problem it is necessary to find the eigenvalues and eigenvectors of the hamiltonian. In this paper we give exact expressions (again in continued fraction form) for these quantities and we discuss the connection between this work and that performed in I. We give explicit expressions for the eigenvectors, eigenvalues and certain transition probabilities in some special cases, and contrast them with the corresponding expressions which would have been obtained if the RWA had been made.

Using a system of units in which $\hbar = 1$, we may write the hamiltonian as

$$H = (\sigma_{3} + \frac{1}{2})\omega_{0} + (a^{\dagger}a + \frac{1}{2})\omega + ga^{\dagger}\sigma_{-} + g^{*}a\sigma_{+} + ga^{\dagger}\sigma_{+} + g^{*}a\sigma_{-}$$
(1)

where ω_0 is the energy difference between the two atomic eigenstates, and ω is the energy of a field quantum. a^{\dagger} and a are the usual creation and annihilation operators for bosons, and σ_+ , σ_- , and σ_3 are the spin one half operators used in I. g is a complex coupling constant.

Hamiltonians of the form (1) are of fairly frequent occurrence in physics, describing, for example, the interaction of a photon or phonon with an effectively two-level system. To give an example of an explicit expression for g, we take the case of an atom interacting

with the electromagnetic field in the electric dipole approximation, when g is given by

$$g = -i \left(\frac{\omega}{2\epsilon_0}\right)^{1/2} \boldsymbol{d} \cdot \boldsymbol{u}$$
⁽²⁾

where d is the dipole matrix element and u is the normal mode function for the field. Although it is the multi-atom, multi-mode generalizations of (1) which are of most interest, it is clearly important to examine the properties of exact solutions of this simple case, if only to provide a check on the validity of approximation treatments. The importance of the single-atom, single-mode model in quantum optics is that it is often used as the starting point for various theories, such as those of the laser and optical/radio-frequency double resonance phenomena.

A common approximation, particularly in quantum optics, is to ignore the final two terms in (1). This is the so-called rotating wave approximation (RWA). Exact solutions of (1) in this case have been given by Jaynes and Cummings (1963). We will frequently make comparison between results obtained using the RWA and our more accurate treatment. Previous work in this area has been performed by Walls (1972) and Agarwal (1971). Walls has used a resolvent technique to calculate the probability of stimulated emission as a function of time. He finds similar results to those obtained using the RWA but with the frequency difference $\omega - \omega_0$ replaced by $\omega - \omega_0 - 2|g|^2/(\omega + \omega_0)$. We obtain a somewhat more complicated result. Agarwal has used a master equation approach to investigate the validity of the RWA, but he was mainly concerned with the N atom, manymode and N oscillator, many-mode problems. He calculated the initial rate of spontaneous emission for these systems, but for the case of a single atom, which is our main concern here, his approximations were such that his expressions reduced to those equivalent to the RWA. Although the RWA is adequate for many physical situations it is not capable of accounting for all the phenomena of double-resonance experiments, for example.

Continued fraction solutions have been obtained for related problems in quantum optics. For example, Autler and Townes (1955), obtained continued fraction solutions to the problem of the Stark effect in rapidly oscillating electric fields. This is similar to the situation we discuss here except that the fields involved in their case were classical. Shirley (1965) has given a discussion of the *formal* analogy between the classical and quantum-mechanical problems. Stenholm and Lamb (1969) have used continued fractions in their discussion of semiclassical laser theory, and Stenholm (1972a, b) has adapted this approach to give an elegant account of double-resonance phenomena. Continued fractions are useful because: (a) it is usually fairly easy to truncate them and so obtain analytical expressions at low orders; and (b) if higher accuracy is required, they are reasonably convenient for numerical work, it being possible to calculate them using an iterative procedure.

In § 2 we derive formal expressions for the eigenvectors and eigenvalues in terms of continued fractions, and in § 3 we discuss the time dependent properties. Explicit expressions are given for the eigenvalues, eigenvectors, and various time dependent transition probabilities in § 4. The rate of convergence of the continued fractions is discussed in § 5.

2. Exact expressions for the eigenvectors and eigenvalues

Let $|\alpha\rangle$ and $|\beta\rangle$ denote the excited and ground states of the atom respectively, and let

 $|n\rangle$ be an eigenvector of the Bose number operator $a^{\dagger}a$. Then using the completeness relations

$$\sum_{n=0}^{\infty} |n\rangle \langle n| = 1 \quad \text{and} \quad |\alpha\rangle \langle \alpha| + |\beta\rangle \langle \beta| = 1,$$
(3)

and ignoring the zero-point energy, we may write the hamiltonian (1) in the form

$$H = \omega_0 |\alpha\rangle \langle \alpha| + \sum_{n=0}^{\infty} |n\rangle n \omega \langle n| + \sum_{n=0}^{\infty} \sqrt{n+1} (|\alpha\rangle \langle \beta| + |\beta\rangle \langle \alpha|) \\ \times (g|n+1\rangle \langle n| + g^*|n\rangle \langle n+1|).$$
(4)

We denote the exact eigenvalues of H by d, the corresponding eigenvectors by $|d\rangle$, and we make the expansion

$$|d\rangle = \sum_{m=0}^{\infty} \left(D_m^{\alpha} |\alpha\rangle + D_m^{\beta} |\beta\rangle \right) |m\rangle$$
(5)

where the coefficients D_m^{α} and D_m^{β} are to be determined. We can obtain equations for the coefficients by operating with (4) on (5); we find

$$H|d\rangle = \sum_{n=0}^{\infty} \{ [\omega_0 D_n^{\alpha} | \alpha \rangle + n\omega (D_n^{\alpha} | \alpha \rangle + D_n^{\beta} | \beta \rangle)] | n \rangle + (D_n^{\alpha} | \beta \rangle + D_n^{\beta} | \alpha \rangle) (g\sqrt{n+1} | n+1 \rangle + g^* \sqrt{n} | n-1 \rangle) \}.$$
(6)

We may replace n by n + 1 in the final term, and n by n - 1 in the penultimate term, without affecting the limits on the sum over n. If this is done, and the terms in $|\alpha\rangle|n\rangle$ and in $|\beta\rangle|n\rangle$ are collected together, we obtain

$$H|d\rangle = \sum_{n=0}^{\infty} \{ [(\omega_0 + n\omega)D_n^{\alpha} + g\sqrt{n}D_{n-1}^{\beta} + g^*\sqrt{n+1}D_{n+1}^{\beta}]|\alpha\rangle|n\rangle + [n\omega D_n^{\beta} + g\sqrt{n}D_{n-1}^{\alpha} + g^*\sqrt{n+1}D_{n+1}^{\alpha}]|\beta\rangle|n\rangle \}.$$
(7)

If $|d\rangle$ is to be an eigenvector of H belonging to the eigenvalue d the right-hand side of (7) must be equal to

$$d|d\rangle \equiv d\sum_{n=0}^{\infty} \left(D_{n}^{\alpha} |\alpha\rangle |n\rangle + D_{n}^{\beta} |\beta\rangle |n\rangle \right).$$
(8)

Equating separately the terms in $|\alpha\rangle|n\rangle$ and $|\beta\rangle|n\rangle$ in the right-hand sides of (7) and (8) we find that the coefficients must satisfy the following simultaneous recurrence relations :

$$(d - \omega_0 - n\omega)D_n^{\alpha} = g\sqrt{n}D_{n-1}^{\beta} + g^*\sqrt{n+1}D_{n+1}^{\beta}$$
(9a)

$$(d - n\omega)D_n^{\beta} = g\sqrt{n}D_{n-1}^{\alpha} + g^*\sqrt{n+1}D_{n+1}^{\alpha}$$
(9b)

for n = 0, 1, 2, 3, ... These equations are the homogeneous forms of the equations (18) and (19) of I; they are also similar to the equations which arise in the problem of a twolevel atom interacting with a classical field (eg Shirley 1965), but in the classical case, n extends over positive and negative integers, and $g\sqrt{n+1}$ and $g\sqrt{n}$ are both equated to the amplitude of the classical field.

The equations (9) in fact generate two independent sets of coupled equations; if one takes n = 0 in (9a) initially, then it is easily verified that the coefficients D_0^{α} , D_1^{β} , D_2^{α} , D_3^{β} , D_4^{α} ,..., are connected, whereas if one begins with n = 0 in (9b) the coefficients

 $D_0^{\beta}, D_1^{\alpha}, D_2^{\beta}, D_3^{\alpha}, D_4^{\beta}, \ldots$, are coupled. We must consider these two sets of equations separately.

If we set |g| = 0, the equations (9) reduce to

$$(d_0 - \omega_0 - n\omega)D_n^a(0) = 0$$
 (10a)

$$(d_0 - n\omega)D_n^{\beta}(0) = 0 \tag{10b}$$

which have the solutions

$$d_0(\alpha, s_1) = \omega_0 + s_1 \omega, \qquad D_n^{\alpha}(0) = \delta_{n, s_1}, \qquad D_n^{\beta}(0) = 0 \qquad (11a)$$

$$d_0(\beta, s_2) = s_2 \omega,$$
 $D_n^{\alpha}(0) = 0,$ $D_n^{\beta}(0) = \delta_{n, s_2},$ (11b)

s = 0, 1, 2, 3, ... It is clear that the eigensolutions are characterized by the quantum numbers α or β and an integer s which determines the number of photons present. The eigenkets corresponding to (11) are

$$|d_0(\alpha, s_1)\rangle = |\alpha\rangle|s_1\rangle \tag{12a}$$

and

$$|d_0(\beta, s_2)\rangle = |\beta\rangle|s_2\rangle \tag{12b}$$

respectively.

Equations (9) determine the energy eigenvalues d in addition to the coefficients D_n^{α} and D_n^{β} . In principle, the eigenvalues could be determined by finding the zeros of the infinite determinant of the system of equations, as in the case of Hill's equation but this is not the approach we employ here. Our technique is to find solutions of (9) which reduce to the unperturbed eigenstates (11) as $|g| \rightarrow 0$. This is done by finding two independent solutions for the coefficients, one applicable for n > s and the other for n < s. Requiring these solutions to match at n = s gives us a condition which determines the eigenvalues.

We now look for solutions of (9) which reduce to (11) when $|g| \rightarrow 0$. Consider first those solutions which reduce to (11*a*): we try the substitutions

$$\left(\frac{g^{n-s}D_{s}^{\alpha}(\alpha,s)}{\mu_{s+1}\lambda_{s+2}\mu_{s+3}\dots\lambda_{n}}\left(\frac{n!}{s!}\right)^{1/2}, \qquad n=s+2, s+4, s+6,\dots$$
(13a)

$$D_n^{\alpha}(\alpha, s) = \begin{cases} P_s + P_s + P_s + 2P_s + 3 + 2P_s + 2P_s + 3 + 2P_s + 3 + 2P_s + 3 + 2P_s + 3 + 2P_s + 2P_s + 3 + 2P_s + 2P_s + 3 + 2P_s + 2$$

and

$$D_{n}^{\beta}(\alpha, s) = \begin{cases} \frac{g^{n-s} D_{s}^{\alpha}(\alpha, s)}{\mu_{s+1} \lambda_{s+2} \mu_{s+3} \dots \mu_{n}} \left(\frac{n!}{s!}\right)^{1/2}, & n = s+1, s+3, \dots \\ \frac{(g^{*})^{s-n} D_{s}^{\alpha}(\alpha, s)}{m_{n} l_{n+1} m_{n+2} \dots m_{s-1}} \left(\frac{s!}{n!}\right)^{1/2}, & n = s-1, s-3, \dots \end{cases}$$
(14a)
(14b)

where the quantities μ_n , λ_n , l_n , m_n are to be determined. As we shall see the coefficient $D_s^{\alpha}(\alpha, s)$, in terms of which all the other coefficients are measured, is fixed by requiring that the eigenvectors be normalized.

Substituting from (13a) and (14a) into (8a), assuming n > s, we find that (11a) and (11b) are solutions providing that

$$\lambda_n = d - \omega_0 - n\omega - \frac{|g|^2(n+1)}{\mu_{n+1}}, \qquad n = s+2, s+4, s+6, \dots$$
(15)

Similarly, putting (13a) and (14a) into (9b) (assuming n > s) leads to

$$\mu_n = d - n\omega - \frac{|\mathbf{g}|^2(n+1)}{\lambda_{n+1}}, \qquad n = s+1, s+3, s+5, \dots$$
(16)

By repeated use of (13) and (14) one finds that the λ_n and μ_n are continued fractions. For example,

$$\lambda_n = d - \omega_0 - n\omega - \frac{|g|^2(n+1)}{d - (n+1)\omega - \frac{|g|^2(n+2)}{d - \omega_0 - (n+2)\omega - \dots}}.$$
(17)

In (15), (16) and (17) the d is understood to stand for the eigenvalue $d(\alpha, s)$ which is yet to be determined.

Likewise, by putting (13b) and (14b) in (9a) and (9b) for n < s, we find that the l_n and m_n are *finite* continued fractions defined by the relations

$$l_n = d - \omega_0 - n\omega - \frac{|g|^2 n}{m_{n-1}}, \qquad n = s - 2, s - 4, s - 6, \dots,$$
(18)

and

$$m_n = d - n\omega - \frac{|g|^2 n}{l_{n-1}}, \qquad n = s - 1, s - 3, s - 5, \dots$$
 (19)

The continued fractions λ_n, μ_n, l_n and m_n also arose in I, where they are discussed in a little more detail.

Putting n = s in (9a) we obtain the relation

$$(d - \omega_0 - s\omega)D_s^{\alpha}(\alpha, s) = \left(\frac{|g|^2 s}{m_{s-1}} + \frac{|g|^2(s+1)}{\mu_{s+1}}\right)D_s^{\alpha}(\alpha, s).$$
(20)

Now $D_s^{\alpha}(\alpha, s)$ is the coefficient of $|\alpha\rangle|s\rangle$ in the expansion (5), and we wish this quantity to be non-zero in the limit $|g| \to 0$; this implies that

$$d(\alpha, s) - \omega_0 - s\omega - \frac{|g|^2 s}{m_{s-1}(d(\alpha, s))} - \frac{|g|^2 (s+1)}{\mu_{s+1}(d(\alpha, s))} = 0.$$
 (21)

This equation determines the energy eigenvalues $d(\alpha, s)$; bearing in mind that $m_{s-1}(d(\alpha, s))$ and $\mu_{s+1}(d(\alpha, s))$ are functions of $d(\alpha, s)$, it follows that it will have an infinite number of roots. For future reference, we denote the function of d on the left-hand side of (21) by $\Lambda_{\alpha,s}(d)$.

The procedure for finding the (β, s) eigensolutions is entirely analogous to that just described for the (α, s) solutions; we make the substitutions

$$\int \frac{g^{n-s} \mathcal{D}_s^{\beta}(\beta, s)}{\lambda_{s+1} \mu_{s+2} \lambda_{s+3} \dots \lambda_n} \left(\frac{n!}{s!}\right)^{1/2}, \qquad n = s+1, s+3, s+5, \dots$$
(22a)

$$D_n^{\alpha}(\beta, s) = \begin{cases} s + 1 + 1 + 2 + 1 + 2 + 1 + 2 + 1 \\ \frac{(g^*)^{s-n} D_s^{\beta}(\beta, s)}{l_n m_{n+1} l_{n+2} \dots l_{s-1}} \left(\frac{s!}{n!}\right)^{1/2}, & n = s-1, s-3, s-5, \dots \end{cases}$$
(22b)

and

$$\sum_{\lambda = 1}^{\beta(\beta, s)} \left\{ \frac{g^{n-s} D_s^{\beta}(\beta, s)}{\lambda_{s+1} \mu_{s+2} \lambda_{s+3} \dots \mu_n} \left(\frac{n!}{s!} \right)^{1/2}, \qquad n = s+2, s+4, s+6, \dots \right\}$$
(23a)

$$D_n^{\beta}(\beta, s) = \begin{cases} \frac{(g^*)^{s-n} D_s^{\beta}(\beta, s)}{m_n l_{n+1} m_{n+2} \dots l_{s-1}} \left(\frac{s!}{n!}\right)^{1/2}, & n = s-2, s-4, s-6, \dots, \end{cases}$$
(23b)

and we find that (22) and (23) are solutions providing that the λ_n , μ_n , l_n and m_n satisfy the same equations as before (ie equations (15), (16), (18) and (19)). By considering the case n = s we find that the (β , s) eigenvalues are determined by the equation

$$d(\beta, s) - s\omega - \frac{|g|^2 s}{l_{s-1}(d(\beta, s))} - \frac{|g|^2 (s+1)}{\lambda_{s+1}(d(\beta, s))} = 0.$$
 (24)

We denote the left-hand side of this expression by $\Lambda_{\beta,s}$.

Although equations (21) and (24) each have an infinite number of roots, they possess properties which greatly simplify the problem of locating these roots. From the way in which we have formulated the problem, it is clear that the root of (21) which tends to $\omega_0 + s\omega$ as |g| tends to zero, and the root of (24) which tends to $s\omega$ as |g| tends to zero, are of special significance; we denote these two roots by d(+, s+1) and d(-, s) respectively. Now, using the definitions of the continued fractions (equations (15), (16), (18), and (19)), one can show straightforwardly that:

(i) if d(s), given as an explicit function of s, satisfies (21), then it also satisfies an equation similar to (21) but with s replaced by $s \pm 2$. As a consequence, it follows that if d(s) is a solution of (21), then $d(s \pm 2n)$ is also a solution of (21), where n is an integer. (It is understood that the argument of $d(s \pm 2n)$ can never be negative.)

(ii) if d(s), given as an explicit function of s, satisfies (21), then it also satisfies an equation similar to (24) but with s replaced by $s \pm 1$. It follows that if d(s) satisfies (21), then $d(s \pm (2n+1))$ satisfies (24).

These two statements also hold if the roles of equations (21) and (24) are interchanged.

We note that d(-, s+1) is also a solution of (21) as |g| tends to zero. It follows that if the eigenvectors are continuous functions of |g| then the roots of (21) are

$$\dots$$
, $d(\pm, s-5)$, $d(\pm, s-3)$, $d(\pm, s-1)$, $d(\pm, s+1)$, $d(\pm, s+3)$, $d(\pm, s+5)$, \dots

and the roots of (24) are

$$\dots, d(\mp, s-4), d(\mp, s-2), d(\mp, s), d(\mp, s+2), d(\mp, s+4), \dots$$

It is clear that the roots, d(+, s) and d(-, s) are fundamental in the sense that once they are known as explicit functions of s then all the roots of (21) and (24) can be generated.

Using (13) and (14) the (α, s) eigenvectors may be written as

$$\begin{aligned} |\alpha, s; d(\alpha, s) \rangle \\ &= D_{s}^{\alpha}(\alpha, s) \bigg[\sum_{n=1}^{int(s/2)} \frac{(g^{*})^{2n-1}(s!/(s-2n+1)!)^{1/2}}{m_{s-2n+1}^{\alpha}l_{s-2n+2} \dots m_{s-1}^{\alpha}} \\ &\times \left(\frac{g^{*}\sqrt{s-2n+1}|s-2n\rangle|\alpha\rangle}{l_{s-2n}^{\alpha}} + |s-2n+1\rangle|\beta\rangle \right) + |\alpha\rangle|s\rangle \end{aligned}$$
(25)
$$&+ \sum_{n=1}^{\infty} \frac{g^{2n-1}((s+2n-1)!/s!)^{1/2}}{\mu_{s+1}^{\alpha}\lambda_{s+2}^{\alpha} \dots \mu_{s+2n-1}^{\alpha}} \left(\frac{g\sqrt{s+2n}|s+2n\rangle|\alpha\rangle}{\lambda_{s+2n}^{\alpha}} + |\beta\rangle|s+2n-1\rangle \right) \bigg]$$

where

$$int(s/2) = \begin{cases} s/2 & \text{if } s \text{ even} \\ (s-1)/2 & \text{if } s \text{ odd} \end{cases}$$

and $m_{s-2n+1}^{\alpha} \equiv m_{s-2n+1}(d(\alpha, s))$ etc. It is clear that $D_s^{\alpha}(\alpha, s)$ is determined by normalization. Our notation for the (α, s) eigenvectors shows explicitly that the (α, s) eigenvectors are functions of the $d(\alpha, s)$ where $d(\alpha, s)$ is any root of (21). The (β, s) eigenvectors would be written $|\beta, s; d(\beta, s)\rangle$ where $d(\beta, s)$ is any root of (24). The corresponding expression for $|\beta, s; d(\beta, s)\rangle$ is obtained by interchanging α and β , λ_n and μ_n , l_n and m_n , in (25).

The $d(\alpha, s)$ which appears in (25) may be any root of (21). It can be shown that if we take $d(\alpha, s) = d(+, s+1\pm 2n)$ in (25), and then take the limit $|g| \rightarrow 0$, we obtain the unperturbed eigenvectors $|\alpha\rangle|s\pm 2n\rangle$, whereas if we take $d(\alpha, s) = d(-, s\pm 2n)$ and then let $|g| \rightarrow 0$, we obtain the unperturbed eigenvectors $|\beta\rangle|s\pm 2n\rangle$. In fact we can show generally that

$$|\alpha, s; d(+, s+1\pm 2n)\rangle = |\alpha, s+1\pm 2n; d(+, s+1\pm 2n)\rangle$$
(26)

and

$$|\alpha, s; d(-, s \pm 2n)\rangle = |\beta, s \pm 2n; d(-, s \pm 2n)\rangle.$$

Thus in order to find all the eigenvalues and all the eigenvectors of H it is necessary to solve either (21) or (24), and substitute the resulting eigenvalues into either $|\alpha, s; d(\alpha, s)\rangle$ or $|\beta, s; d(\beta, s)\rangle$. (21) and (24), and $|\alpha, s; d(\alpha, s)\rangle$ and $|\beta, s; d(\beta, s)\rangle$ are formally equivalent, although one member of the pair may be more convenient to use in practice than the other. It is clear that the eigenvectors are characterized completely by the eigenvalues, so in future we will write

$$|\gamma, s; d(\gamma, s)\rangle \equiv |d(\gamma, s)\rangle, \qquad \gamma = \alpha \text{ or } \beta.$$

3. The time dependent properties

In I we have obtained expressions for the time dependent conditional probabilities $P_{\delta,n}^{\gamma,s}(t)$ where $P_{\delta,n}^{\gamma,s}(t)$ is the probability that the system will be in the state $|\delta\rangle|n\rangle$ at time t if it was in the state $|\gamma\rangle|s\rangle$ at time 0. $|\gamma\rangle$ and $|\delta\rangle$ label states of the atom, and $|n\rangle$ and $|s\rangle$ denote states of the field in which there are n and s photons present respectively. The expressions obtained were of the form

. . . .

$$P_{\delta,n}^{\gamma,s}(t) = \left| \frac{-1}{2\pi i} \oint dx \, e^{-ixt} L_{\delta,n}^{\gamma,s}(x) \right|^2 \tag{27}$$

where

$$L_{\alpha,n}^{\gamma,s}(x) = \begin{cases} \frac{g^{n-s}(n!/s!)^{1/2}}{\lambda_n\mu_{n-1}\dots(\lambda_{s+1} \text{ or } \mu_{s+1})\Lambda_{\gamma,s}}, \\ n = s+2, s+4, s+6, \dots, \text{ if } \gamma = \alpha, \text{ and} \\ n = s+1, s+3, s+5, \dots, \text{ if } \gamma = \beta \\ \frac{(g^*)^{s-n}(s!/n!)^{1/2}}{m_{s-1}l_{s-2}\dots(l_n \text{ or } m_n)\Lambda_{\gamma,s}}, \\ n = s-2, s-4, s-6, \dots, \text{ if } \gamma = \alpha, \text{ and} \\ n = s-1, s-3, s-5, \dots, \text{ if } \gamma = \beta \end{cases}$$
(29)

where $\gamma = \alpha$ or β . To obtain the corresponding expressions for $L_{\beta,n}^{\gamma,s}(x)$ replace the λ 's by the μ 's and vice versa, and the *l*'s by the *m*'s and vice versa, in (28) and (29). $\Lambda_{\gamma,s}(x)$ is the function on the left-hand side of (21) if $\gamma = \alpha$ and on the left-hand side of (24) if $\gamma = \beta$. The sequence $\lambda_n \mu_{n-1} \lambda_{n-2} \dots$ in (28) terminates in μ_{s+1} if n-s is even, and in λ_{s+1} if n-s is odd. A similar interpretation applies to (29).

These results may be cast into a more symmetric form by making use of the relation

$$\Lambda_{\alpha,s} = \frac{\lambda_{s}\mu_{s-1}\lambda_{s-2}\dots(\lambda_{0} \text{ or } \mu_{0})}{m_{s-1}l_{s-2}m_{s-3}\dots(l_{0} \text{ or } m_{0})}$$
(30)

which is easily established using the definitions (21) for $\Lambda_{\alpha,s}$, and (16), (17), (18) and (19) for the continued fractions. The sequences in (30) terminate in λ_0 and m_0 if s is even and in μ_0 and m_0 if s is odd. A similar relationship holds for $\Lambda_{\beta,s}$ but with λ_n and μ_n , l_n and m_n interchanged. Using (30) in (28) and (29) we may show, for example, that

$$L_{\alpha,n}^{\alpha,s}(x) = (L_{\alpha,n}^{\alpha,n}(x))^* = g^{n-s} \left(\frac{n!}{s!}\right)^{1/2} \frac{m_{s-1}l_{s-2}\dots(l_0 \text{ or } m_0)}{\lambda_n \mu_{n-1}\dots(\lambda_0 \text{ or } \mu_0)}, \qquad n = s+2, s+4, \dots \quad (31)$$

$$L_{\alpha,n}^{\beta,s}(x) = (L_{\beta,s}^{\alpha,n}(x))^* = g^{n-s} \left(\frac{n!}{s!}\right)^{1/2} \frac{l_{s-1}m_{s-2}\dots(m_0 \text{ or } l_0)}{\lambda_n\mu_{n-1}\dots(\mu_0 \text{ or } \lambda_0)}, \qquad n = s+1, s+3,\dots$$
 (32)

Similar relations hold for $L^{\beta,s}_{\beta,n}(x)$ and for the situation in which n < s. The symmetry relation

$$P_{\delta,n}^{\gamma,s}(t) = P_{\gamma,s}^{\delta,n}(t) \tag{33}$$

obviously follows.

Now in I it was shown that the poles of $L_{\delta,n}^{\gamma,s}(x)$ determine the exact eigenvalues of H, whereas in the present paper we have shown that they are determined by the zeros of $\Lambda_{\gamma,s}(x) = 0$. Comparison of (30), (31) and (32) makes it plausible that these two prescriptions for finding the eigenvalues are equivalent.

An alternative way of developing the time dependent theory would be to expand the state $|\gamma, s\rangle$ in terms of the basic vectors $|d\rangle$, and then to pick out the component in $|\delta\rangle|n\rangle$. The treatment given in I is more succinct.

4. Explicit case: comparisons with the rotating wave solutions

4.1. The case of resonance

A special case occurs if the atom and the field mode are resonant, for then $\omega = \omega_0$, and the two fundamental eigenvalues become equal. For the case of equation (21),

$$d(+, s+1) \rightarrow d(-, s+1) \rightarrow (s+1)\omega$$
 as $|g| \rightarrow 0$.

The resonant situation is a particularly simple one to discuss, as the properties of the system are now functions of only three variables $s, \gamma = g/\omega$, and $\tau = \omega t$. Let us assume

$$|\gamma|\sqrt{s+1} \ll 1,\tag{34}$$

and make a series expansion for the fundamental roots in powers of $|\gamma|$. It is easily found that

$$d(\pm, s+1) = \omega[s+1\mp |\gamma|\sqrt{s+1} - \frac{1}{2}|\gamma|^2 \pm \frac{1}{8}|\gamma|^3(s+1)^{3/2} - \frac{1}{4}|\gamma|^4(s+1)^2 \dots].$$
(35)

The third term, $-\frac{1}{2}|y|^2$ which is the same for all eigenvalues, merely represents a shift

in the datum point for measuring energies; the other terms involving powers of $|\gamma|$ represent self-energy terms of the sort which give rise to the Lamb shift and the Bloch-Siegert shift.

We note that the RWA (see eg Swain 1972) gives only the first two terms in (35), so that, at resonance, the RWA is correct only to first order in $|\gamma|$. It is in the resonant situation that the RWA should be most accurate.

Evaluating the unnormalized fundamental eigenvectors using (35) and (25) correct to second order in $|\gamma|^2$ gives

$$\begin{aligned} |d(\pm,s+1)\rangle \\ &= \frac{(\gamma^*)^2}{4} \sqrt{s(s+1)} |\alpha\rangle |s-2\rangle + \frac{\gamma^* \sqrt{s}}{2(1 \mp \frac{1}{2}|\gamma| \sqrt{s+1})} |\beta\rangle |s-1\rangle \\ &+ |\alpha\rangle |s\rangle \mp \frac{\gamma |\beta\rangle |s+1\rangle}{|\gamma|(1 \pm \frac{1}{2}|\gamma| \sqrt{s+1} + \frac{1}{8}|\gamma|^2 (s+3))} \pm \frac{\gamma \sqrt{s+2}}{2} |\alpha\rangle |s+2\rangle \end{aligned}$$

$$\mp \frac{\gamma^2 \sqrt{(s+2)(s+3)}}{4} |\beta\rangle |s+3\rangle. \tag{36}$$

We note that in this expression the two unperturbed eigenstates $|\alpha\rangle|s\rangle$ and $|\beta\rangle|s\rangle$ have approximately equal weighting. In the limit, $|\gamma| \rightarrow 0$ the states $|d(+, s+1)\rangle$ and $|d(-, s+1)\rangle$ become degenerate, and the eigenvectors become

$$|d(\pm, s+1)\rangle \rightarrow |\alpha\rangle|s\rangle \mp \frac{\gamma}{|\gamma|}|\beta\rangle|s+1\rangle, \tag{37}$$

which are the states normally used as basis states in ordinary degenerate perturbation theory. They are also the exact eigenstates of the rotating wave hamiltonian at resonance, so that the RWA gives the eigenstates of (1) correct to zeroth order only.

We may also calculate the time dependent properties. Consider first transitions from the unperturbed state $|\alpha\rangle|s\rangle$ to the states shown in figure 1(*a*). The transition probability from $|\alpha\rangle|s\rangle$ to any of these states has an amplitude of γ^2 or larger. Consider first the calculation of $P_{\alpha,s}^{\alpha,s}(t)$. According to (28), (16) and (19),



Figure 1. The transitions which have amplitudes of the order of γ^2 or larger.

where $\epsilon = x/\omega$. This has poles near $\epsilon = s+1, s-1, s+3, \ldots$, the precise positions of which are given by (35) on taking the appropriate sign and value of s. The integral in (27) may be evaluated using the calculus of residues, when we find, to second order in $|y|^2$,

$$P_{\alpha,s}^{a,s}(t) = \left[1 - \frac{1}{2}|\gamma|^2 s\right] - \left[1 - \frac{1}{4}|\gamma|^2 (3s+1)\right] \sin^2(\theta_{s+1}\tau) + \frac{1}{2}|\gamma|^2 s \cos(\theta_{s+1}\tau) \cos(\theta_{s-1}\tau) \cos(2\tau)$$
(39)

where

$$\theta_s = |\gamma| \sqrt{s(1 - \frac{1}{8}|\gamma|^2 s)}.$$
(40)

We may proceed in a similar fashion to find the probabilities of the other transitions shown in figure 1(a). For these, we find

$$P_{\beta,s+1}^{\alpha,s}(\tau) = \left[1 - \frac{3}{4}|\gamma|^2(s+1)\right]\sin^2(\theta_{s+1}\tau)$$
(41)

$$P_{\alpha,s+2}^{\alpha,s}(\tau) = \frac{1}{4} |\gamma|^2 (s+2) \sin^2(\theta_{s+1}\tau)$$
(42)

$$P_{\alpha,s-2}^{\alpha,s}(\tau) = \frac{1}{4}|\gamma|^2 s \sin^2(\theta_{s-1}\tau)$$
(43)

$$P_{\beta,s-1}^{\alpha,s}(\tau) = \frac{1}{2}|\gamma|^2 s\{1 - \frac{1}{2}[\sin^2(\theta_{s+1}\tau) + \sin^2(\theta_{s-1}\tau)] - \cos(\theta_{s+1}\tau)\cos(\theta_{s-1}\tau)\cos 2\tau\}.$$
 (44)

In a typical experiment, the higher frequency terms such as the final terms in (39) and (44) would be averaged to zero. If the quantity being measured was the transition probability from atomic state $|\alpha\rangle$ to $|\beta\rangle$ this would be given by

$$\overline{P^{\alpha}_{\beta}(\tau)} = \overline{P^{\alpha,s}_{\beta,s+1}(\tau)} + \overline{P^{\alpha,s}_{\beta,s-1}(\tau)} \simeq \frac{1}{2}|\gamma|^2 s + (1 - \frac{5}{4}|\gamma|^2 s)\sin^2(\theta_s \tau)$$

where we have assumed $s \gg 1$ and the bar indicates that high frequency contributions have been omitted. This expression is consistent with the low frequency terms of Shirley's (1965) semi-classical treatment.

In the RWA, the corresponding expressions are

$$P_{\alpha,s}^{\alpha,s}(\mathbf{RWA};\tau) = 1 - \sin^2(|\gamma|\sqrt{s+1}\tau)$$
(45)

$$P^{\alpha,s}_{\beta,s+1}(\mathrm{RWA};\tau) = \sin^2(|\gamma|\sqrt{s+1}\tau)$$
(46)

$$P_{\alpha,s\pm 2}^{\alpha,s}(\tau) = P_{\beta,s-1}^{\alpha,s}(\tau) = 0 \tag{47}$$

which are correct only to first order in $|\gamma|$.

In a similar fashion, for the transitions from the state (β, s) indicated in figure 1(b) we find

$$P_{\beta,s}^{\theta,s}(\tau) = \left[1 - \frac{1}{2}|\gamma|^2(s+1)\right] - \left[1 - \frac{1}{4}|\gamma|^2(s+2)\right]\sin^2(\theta_s \tau) + \frac{1}{2}|\gamma|^2(s+1)\cos(\theta_s \tau)\cos(\theta_{s+3}\tau)\cos(2\tau)$$
(48)
$$P_{\alpha,s-1}^{\theta,s}(\tau) = \left(1 - \frac{3}{4}|\gamma|^2s\right)\sin^2(\theta_s \tau)$$
(49)

$$P_{\beta,s+2}^{\beta,s}(\tau) = \frac{1}{4} |\gamma|^2 (s+1) \sin^2(\theta_{s+3}\tau)$$
(50)

$$P_{\beta,s-2}^{\beta,s-2}(\tau) = \frac{1}{4} |\gamma|^2 (s-1) \sin^2(\theta_s \tau)$$
(51)

and

$$P_{\alpha,s+1}^{\theta,s}(\tau) = \frac{1}{2}|\gamma|^2(s+1)\{1 - \frac{1}{2}[\sin^2(\theta_s\tau) + \sin^2(\theta_{s+3}\tau)] - \cos(\theta_s\tau)\cos(\theta_{s+3}\tau)\cos(2\tau)\}.$$
 (52)

From (44) and (52) we see that $P_{\beta,s}^{\alpha,s+1}(\tau) = P_{\alpha,s+1}^{\beta,s}(\tau)$ as required by (33). The corresponding expressions for $P_{\beta,s}^{\beta,s}(\tau)$ and $P_{\alpha,s-1}^{\beta,s}(\tau)$ in the RWA are given by expressions similar to (45) and (46) respectively but with the arguments of the sine functions changed from $|\gamma|\sqrt{s+1}$ to $|\gamma|\sqrt{s}$.

4.2. The general case

It is not difficult to derive expressions for the eigenvalues which are valid off resonance using a process of successive approximation. The simplest, non-trivial approximation to the eigenvalues is the RWA, which gives

$$d(\mathbf{RWA}; \pm, s+1) = s\omega + \frac{1}{2}(\omega + \omega_0) \mp U$$
(53)

where

$$U = [\delta^2 + |g|^2 (s+1)]^{1/2}, \qquad \delta = \frac{1}{2} (\omega - \omega_0).$$
(54)

One may then use this expression in the eigenvalue equation (21) to obtain an expression valid to higher order in |g|, and so on. For example, correct to third order in |g|, we find

$$d(\pm, s+1) = s\omega + \frac{1}{2}(\omega + \omega_0) + \frac{|g|^2}{2} \left(\frac{s}{\Omega \mp U} - \frac{s+2}{\Omega \pm U} \right) \mp V_{\pm}$$
(55)

where

$$V_{\pm} = \left\{ \left[\delta - \frac{|g|^2}{2} \left(\frac{s}{\Omega \mp U} + \frac{s+2}{\Omega \pm U} \right) \right]^2 + |g|^2 (s+1) \right\}^{1/2}$$
(56)

and

$$\Omega = \frac{1}{2}(\omega_0 + 3\omega) \tag{57}$$

It is interesting to note that (55) is of the same form as (53) but with the ω and ω_0 replaced by the effective values

$$\omega \to \omega^* = \omega - \frac{|g|^2(s+2)}{\Omega \pm U}$$
(58)

and

$$\omega_0 \to \omega_0^* = \omega + \frac{|\mathbf{g}|^2 s}{\mathbf{\Omega} \mp U} \tag{59}$$

everywhere except in the $s\omega$ term on the right-hand side of (53).

At resonance, (55) reduces to the first four terms of (35), ie it gives $d(\pm, s+1)$ at resonance correct to third order in $|\gamma|$, whilst well off resonance, ie for $\delta^2 \gg |g|^2(s+1)$, it gives

$$d(+, s+1) = s\omega + \omega_0 - \frac{|g|^2(s+1)}{\omega - \omega_0} + \frac{|g|^2s}{\omega + \omega_0} + O(|g|^4)$$
(60)

$$d(-, s+1) = (s+1)\omega + \frac{|g|^2(s+1)}{\omega - \omega_0} - \frac{|g|^2(s+2)}{\omega + \omega_0} + O(|g|^4),$$
(61)

the usual non-degenerate second-order perturbation theory results. The expansion of (54) in (53) gives only the first two terms of (60) and (61).

(60) and (61) may be used to find the positions of the multiple quantum transitions which occur in radio-frequency spectroscopy (see eg Stenholm 1972a, b and references given therein). The time averaged transition probability, $\overline{P}_{\beta,s+2k+1}^{\alpha,s}$, where k is a positive integer, is a maximum when the parameters are so chosen that |d(+, s) - d(-, s+2k+1)| is a minimum. Replacing s by s+2k in (61) and subtracting the result from (60), we find that the minimum occurs (to this level of approximation the minimum is zero) when

$$\omega_0 = (2k+1)\omega \left(1 - \frac{|g|^2(s+1)}{k(k+1)\omega^2}\right), \qquad k > 1$$

In arriving at this well known result we have put $\omega_0 \simeq (2k+1)\omega$ in the denominations of (60) and (61). This is an example of a situation in which the rotating and anti-rotating terms in the hamiltonian (1) give approximately equal contributions.

It is straightforward to proceed to obtain expressions for the remaining transition probabilities as before, but as the general method is clear, and the resulting expressions cumbersome, we will give just one example, $P_{\beta,s+1}^{\alpha,s}(\tau)$. Assuming that the dominant contribution comes from the poles at d(+, s+1) and d(-, s+1) we find that

$$P_{\beta,s+1}^{\alpha,s}(t) = \frac{|g|^2(s+1)}{R^2} \left(1 + \frac{4|g|^2 U^2 \omega}{R(\Omega^2 - U^2)^2} \right) \sin^2 \left[\left(\frac{V_+ + V_-}{2} - \frac{|g|^2 U(s+1)}{\Omega^2 - U^2} \right) t \right]$$
(62)

where

$$R = V_{+} + \frac{|g|^{2}}{2} \left(\frac{s(U-\delta)}{(\Omega+U)^{2}} + \frac{(s+2)(U+\delta)}{(\Omega-U)^{2}} \right).$$
(63)

For ω close to ω_0 this simplifies to

$$P_{\beta,s+1}^{\alpha,s}(t) = \frac{|g|^2(s+1)\sin^2(\{1-[|g|^2(s+1)/(\omega+\omega_0)^2]\}[\Delta^2+|g|^2(s+1)]^{1/2}t)}{\{[\Delta^2+|g|^2(s+1)]^{1/2}+[|g|^3(s+1)^{3/2}/(\omega+\omega_0)^2]\}^2}$$
(64)

where

$$\Delta = \delta - \frac{|\mathbf{g}|^2 (s+1)}{\omega + \omega_0}.$$
(65)

Other poles give rise to contributions with amplitudes of order $|\gamma|^4$ or smaller.

Expressions analogous to (64) were first derived by Bloch and Siegert (1940) for the case of a spin of one half subjected to a classical oscillating magnetic field. The argument of the sine function in (64) is a minimum when $\Delta = 0$, ie when

$$\omega_{0} = \omega - \frac{2|g|^{2}(s+1)}{\omega + \omega_{0}} \simeq \omega - \frac{|g|^{2}(s+1)}{\omega} \simeq \omega [1 - |\gamma|^{2}(s+1)].$$
(66)

In the RWA, the condition (66) becomes simply $\omega = \omega_0$, and the shift in (66) from this value is referred to as the Bloch-Siegert shift in the classical case. Because our calculation is fully quantum mechanical, our expression for the Bloch-Siegert shift includes the effects of spontaneous emission. We note that the Bloch-Siegert condition (66) is equivalent to

$$\omega_0^* = \omega^*$$

if ω^* and ω_0^* are evaluated correct to second order in $|g|^2$; ie, it is the condition for resonance of the effective frequencies defined in (58) and (59). (66) is also the condition which makes d(+, s+1) - d(-, s+1) a minimum.

The condition (66) has also been derived by Walls (1972), but his expression for $P_{\beta,s+1}^{\alpha,s}(t)$ namely

$$P_{\beta,s+1}^{\alpha,s}(t) = \frac{|g|^2(s+1)}{|g|^2(s+1) + \Delta^2} \sin^2[\Delta^2 + |g|^2(s+1)]^{1/2}t$$
(67)

differs from ours. Walls used a resolvent method, and the discrepancy between his results and ours may be traced to his having used a less accurate expression for the poles of the resolvent than that given by (55).

In the RWA an expression similar to (67) is obtained but now Δ is given by $\Delta = \delta$ rather than by (65). We can obtain the RWA result from (64) and (65) by neglecting the terms in $|g|^2/(\omega + \omega_0)$.

5. Convergence of the continued fractions

In previous sections we have truncated the continued fractions so as to obtain analytic expressions; in this section we consider the validity of the approximations involved by comparing the results obtained for the eigenvalues and transition probabilities by taking the second, third, and fourth approximants to the continued fractions which occur. As we are only interested in testing the rates of convergence, we consider the simplest cases, namely we find the roots of $\Lambda_{\alpha,0} \equiv \lambda_0 = 0$ and we calculate $P_{\alpha,0}^{\alpha,0}(\tau)$ for the three cases, $|\gamma|^2 = 0.1$, $\omega/\omega_0 = 1$, $|\gamma|^2 = 0.1$, $\omega/\omega_0 = 1.2108$ and $|\gamma|^2 = 1$, $\omega/\omega_0 = \frac{5}{3}$. We emphasize that the values of $|\gamma|^2$ are chosen solely to test the rate of convergence and do not correspond to physically realizeable situations. (In quantum optics, for example, typically $|\gamma|^2 \sim 6 \times 10^{-15}/(\omega V)$ where V is the volume of the system (in MKS units) and we assume $\omega \sim \omega_0$.) We have taken the s = 0 case for simplicity; we are not attempting to construct a theory of spontaneous emission which of course would require a many mode model. The values of ω/ω_0 in the last two cases are chosen in such a way as to make $P_{\alpha,0}^{\alpha,0}$ (RWA, τ) oscillate between 1 and 0.1.

In table 1 we have displayed the positions of the roots of $\lambda_0 = 0$ (measured in units of ω_0) for the three values of $|\gamma|^2$ and ω/ω_0 considered. (The first approximant to $\lambda_0 = 0$ has two roots, the second three roots, and so on.) In the first two cases, $|\gamma|^2 = 0.1$ and $\omega/\omega_0 = 1$ and 1.2108, the differences between the first and second approximants for the first two roots is significantly larger than the differences between the second and higher approximants. The convergence of the third and fourth roots is slower, but their effect on the transition probabilities is of lower order than the effect of the first two roots. In the third case considered, $|\gamma|^2 = 1$ and $\omega/\omega_0 = \frac{5}{3}$ the convergence of all the roots is slow.

Similar effects are seen in figures 2 and 3, which show $P_{\alpha,0}^{\alpha,0}(\tau)$ as a function of τ for $|\gamma|^2 = 0.1$ and $\omega/\omega_0 = 1$ and 1.2108 respectively; there is a significant difference between the first and second approximants, but an almost imperceptible difference between the second and higher ones. In figure 4, we see that the differences between all four approximants considered are appreciable. In figures 3 and 4 it is apparent that the more accurate solutions swing closer to zero than the RWA solutions. Also the rate of transfer of energy between the atom and the field is retarded as compared with the RWA.

γ	$\frac{\omega}{\omega_0}$	Approximants			
		1st	2nd	3rd	4th
0.1	1	0.6838	0.6386	0.6359	0.6358
		1.3162	1.2638	1.2588	1.2585
			3.0976	2.5169	2-4276
			_	3.5883	3-4834
		-	_		5·1947
0.1	1.2108	0.7721	0.7446	0.7434	0.7437
		1.4387	1.3777	1.3738	1.3737
			3.5101	3.0335	2.9679
				4.1141	4.0037
		-		_	6-0194
1.0	1.6667	0.2793	0.0928	0.0588	0.05408
		2.3874	1.9220	1.7623	1.7127
			4.9853	3-5661	3.1552
				6.6129	5.8334
			_		8.9116

Table 1. The zeros of λ_0 calculated in the first, second, third and fourth approximants as functions of γ and ω/ω_0



Figure 2. Plot of $P_{x,0}^{z,0}(\tau)$ against τ for $\gamma^2 = 0.1$ and $\omega = \omega_0$. The full curve is the first approximant (RWA), the broken curve is the second approximant and the full circles are the third approximant. The difference between the third and fourth approximants is indiscernible in this diagram.

We would expect the rates of convergence to be determined mainly by the value of $|\gamma|^2(s + 1)$ in the general case, eg we would expect little difference between the rates of convergence of the probabilities $P_{\alpha,s}^{\alpha,s}(\tau)$ and $P_{\alpha,s}^{\alpha,s'}(\tau)$ if $|g|^2(s+1) \simeq |g'|^2(s'+1)$ and $\omega' = \omega$, $\omega'_0 = \omega_0$. Now the case we have examined (s = 0) is a special case in that high frequency terms such as the final term in (39) are excluded; nevertheless, we would not expect this to affect significantly the rate at which successive approximants converge. Thus for example we would expect the second approximant to be adequate if the condition $|\gamma|^2(s+1) \lesssim 0.1$ is satisfied. Stenholm (1972b) has discussed the rate of convergence of continued fractions akin to ours for $|\gamma|^2(s+1) \gtrsim 1$.



Figure 3. Plot of $P_{\alpha,0}^{*,0}(\tau)$ against τ for $\gamma^2 = 0.1$ and $\omega = 1.2108\omega_0$. The full curve is the first approximant (RWA), the broken curve is the second approximant and the full circles are the third approximant. The third and fourth approximants differ significantly only in the final two points shown.



Figure 4. Plot of $P_{a,0}^{*,0}(\tau)$ against τ for $\gamma^2 = 1.0$ and $\omega = 1.6667\omega_0$. Full curve: first approximant (RwA); broken curve: second approximant; full circles: third approximant; chain curve: fourth approximant.

For the case of the interaction of a quantized field mode with a two-level atom, the interaction constant is given by (2). Assuming a value for $\mu \sim 3.33 \times 10^{-30}$ Cm, and that the electromagnetic radiation is incident upon a cell of surface area 10^{-4} m² we find

$$|\gamma|^2(s+1) \sim \frac{2W}{\omega^2} \times 10^{15}$$

where W is the laser power in watts. Clearly for optical frequencies, $\omega \sim 10^{15}$ Hz, $|\gamma|^2(s+1)$ will be very small for currently accessible maximum intensities, but at lower frequencies, eg $\omega \sim 10^9$ Hz, there should be little difficulty in making $|\gamma|^2 s$ an appreciable fraction of one. In this case the value of s will be so large that the effects of spontaneous emission will be negligible.

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