Line-shape function for the microwave-induced hyperfine-level transition in positronium

F. H. M. Faisal and P. S. Ray
Fakultät für Physik, Universität Bielefeld, 4800 Bielefeld 1, Federal Republic of Germany
(Received 17 September 1982; revised manuscript received 26 June 1984)

Recently (e.g., Rich, 1981; Mills, 1983) it has been realized that the effect of the annihilation width on microwave absorption line shape for the Zeeman transitions between the hf levels of the Ps atom in its ground state has to be accounted for at a better level of approximation than it has been in the past. In the traditional Breit-Rabi representation the subtle effects of the annihilation widths show up as an extra off-diagonal coupling between the off-resonant and one of the near-resonant states. In this paper we derive an analytical line-shape formula by solving the rotating-wave amplitude equations within the BR representation, where the off-resonant off-diagonal coupling is treated by the adiabatic-elimination procedure. The resulting line shape is found to be slightly asymmetric in form—a conclusion which has been first reached by Mills (1983). It is seen explicitly that due to the off-diagonal coupling an effective decay constant is dependent on the microwave frequency (ω). It is also shown that only if, as a zeroth approximation, this ω dependence is neglected, then a formula for the hyperfine interval ΔW, recently given by Rich (1981) on the basis of heuristic arguments, may be obtained. Explicit illustrations of the present slightly asymmetric line-shape function, and the ω dependence of the said effective decay constant $[\Lambda_{1,0}(\omega)]$ are also presented. We have taken this opportunity to point out certain apparent discrepancies noted among some of the previous line-shape formulas.

I. INTRODUCTION

The theoretical QED calculation of the energy difference between the triplet and the singlet components of the positronium atom in its ground state and their comparison with the experimental measurements have attracted renewed attention recently.[1,2] The theoretical value of the energy difference is known (exactly) up to the fifth power of the fine-structure constant.[3] Experimentally it has been measured with increasing precision over the years.[1,4–6] At the current level of experimental accuracy, and in view of the possibility of calculation of the α^6 terms for ΔW, it is expected that comparison of theory and measurement at the level of a few ppm will be possible in the near future.

Due to the impractically high microwave power needed one cannot observe the direct transition between the $1\,^3S_1$ and $^1S_0$ states. In these experiments, therefore, one first splits the triplet level by applying a static magnetic field and subsequently induces a resonance transition between these perturbed hyperfine levels by tuning a microwave field appropriately.[4] The experimental value for the energy difference $\Delta W(^3S_1-{}^1S_0)$ is then extracted by fitting a theoretical line-shape function to the observed microwave-absorption spectrum. Nevertheless the analysis of the spectral line shape has been made until very recently[7,8,13] without properly accounting for the annihilation effects.

Basic to the derivation of the absorption line shape is the treatment of the Schrödinger equation for the amplitudes of the hyperfine levels in an external microwave field. The original analysis in this context is due to Halpern[9] and Theriot *et al.*,[10] who obtained the first line-shape function explicitly in analyzing their experimental data. Let λ_0 $(=\lambda_{3\gamma})$ and λ_p $(=\lambda_{2\gamma})$ be the annihilation widths of the ortho and para Ps in its ground state $(n=1)$. The complex unperturbed energy values including these widths are then $E_1=W_1-i(\hbar/2)\lambda_0$ and $E_0=W_0-i(\hbar/2)\lambda_p$, respectively, where W_1 and W_0 are the usual real energies of the corresponding states. The splitting of these states by a static magnetic field of strength B_0 parallel to the z axis is depicted schematically (Fig. 1). The Hamiltonian of the perturbed system is given by

$$H=H_A+H_M\ , \tag{1}$$

where H_A is the unperturbed Hamiltonian of the atom and H_M is the interaction of the magnetic field with the system. Explicitly

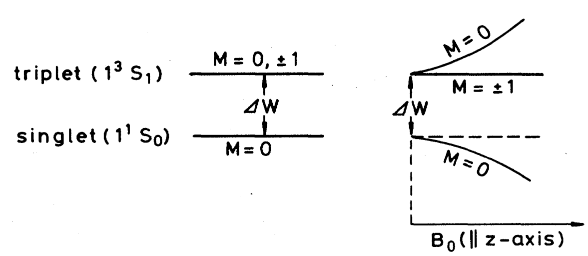

FIG. 1. Splitting of the singlet and triplet ground-state components in the presence of a static magnetic field. The field strength is B_0 and the direction is taken to be parallel to the z axis.

$$H_M=\mu_B g_- \vec{s}_- \cdot \vec{B}_0+\mu_B g_+ \vec{s}_+ \cdot \vec{B}_0$$
$$=\frac{\hbar}{2}\mu_B g(\sigma_z^{(-)}-\sigma_z^{(+)})B_0 \ , \qquad (2)$$

where $\mu_B=e\hbar/2mc$ is the Bohr magneton, $g_-=g_+=g\simeq 2$ the g factor, and $(\vec{s}_-,\vec{s}_+)$ the respective spin vectors of the electron and the positron. In terms of the Pauli spin operators one has $\vec{s}=(\hbar/2)\vec{\sigma}$. Let p be the matrix element of the magnetic perturbation between the unperturbed states:

$$p=\langle {}^3S_1{:}M=0\,|\,H_M\,|\,{}^1S_0{:}M=0\rangle=\hbar\mu_B g B_0 \ .$$

The other matrix elements of H_M between ${}^3S_1$ with $M=\pm 1$ and ${}^1S_0$ with $M=0$ vanish. Thus the magnetic field leaves $M=\pm 1$ components of the triplet state unaltered. Taking into account the annihilation widths, the perturbed (complex) energy eigenvalues have been obtained by Rich[1] as the solution of the secular equation ($\hbar=1$)

$$\det\begin{vmatrix} W_1-i\dfrac{\lambda_0}{2}-E & p \\ p & W_0-i\dfrac{\lambda_p}{2}-E \end{vmatrix}=0 \ . \qquad (3)$$

Writing $\Delta W=W_1-W_0$, $\lambda_+=(\lambda_0+\lambda_p)/2$, $\lambda_-=(\lambda_p-\lambda_0)/2$, the energy eigenvalues are

$$E'_{1,0}=\frac{W_1+W_0}{2}-i\frac{\lambda_+}{2}$$
$$\pm\frac{\Delta W}{2}(1+x^2-y^2+i2y)^{1/2} \ , \qquad (4)$$

where the upper sign goes with E'_1 and the lower sign with E'_0, $x=2\mu_B g B_0/\Delta W$, $p=(x/2)\Delta W$, and $y=\lambda_-/\Delta W$.

Rich[7] has recently utilized the complex eigenvalues which are obtained in the presence of annihilation, to derive in a heuristic manner a correction of the line center with respect to the usual Breit-Rabi formula.[6,10] He gives the correction in hyperfine interval in the form

$$\frac{\Delta W-\Delta W^{\mathrm{BR}}}{\Delta W}=\frac{1}{2}\left[\frac{qx}{1+x^2}\right]^2\frac{(1+x^2)^{1/2}}{(1+x^2)^{1/2}-1} \ , \qquad (5)$$

where ΔW is the actual hyperfine separation ($\Delta W=h\Delta\nu$) and ΔW^{BR} is the experimentally extracted value for ΔW using the Breit-Rabi formula, and the entity q is defined as

$$q=\frac{\lambda_p-\lambda_0}{4\pi\nu}\simeq 3.1\times 10^{-3} \ .$$

The utilization of the change in the eigenvalues of the static problems alone may not provide a proper extraction of ΔW (as noted already by Rich[7]), since inclusion of decay in the static case may also alter the line shape in the presence of the microwave field. Indeed Mills,[8] who formulated the line-shape problem in terms of a set of Liouville equations of the system and obtained the line-shape correction numerically, showed that the line shape to be slightly asymmetrical. He used the numerical line shape so obtained to correct the experimental values of ΔW, extracted previously on the basis of simpler symmetric line shapes, of Mills and Bearman[11] and Egan *et al.*[5] It is interesting to note that the corrections to ΔW thus obtained by Mills and the heuristic estimates of Rich,[7] which are compared in the table below, differ but slightly:

$\Delta W^{\mathrm{expt}}/2\pi$ (MHz)	$\Delta W/2\pi$ (Rich, Ref. 7)	$\Delta W/2\pi$ (Mills, Ref. 8)
203 387.0 (Ref. 11)	203 388.7	203 387.5
203 384 (Ref. 12)	203 385.9	
203 384.9 (Ref. 5)	203 386.8	203 389.0

An independent derivation of the line-shape function, in an analytical form, which includes the effect of off-diagonal decay terms is expected to be helpful in this context. We derive such a spectrum which shows that the line shape is indeed asymmetric as found by Mills. It also clarifies under what approximation a heuristic formula like that of Rich [Eq. (5)] may be obtained.

II. SCHRÖDINGER EQUATION IN BREIT-RABI REPRESENTATION WITH OFF-DIAGONAL DECAY TERMS

The full Schrödinger equation including the decay for the two-level system is given by ($\hbar=1$)

$$H\,|\,\psi(t)\rangle=i\frac{\partial}{\partial t}\,|\,\psi(t)\rangle \ , \qquad (6)$$

where the total Hamiltonian is given as follows:

$$H=H_A-\frac{i}{2}\lambda+H_s+H_D(t) \ . \qquad (7)$$

Here H_A represents as before the Hamiltonian of the Ps atom, λ is the decay matrix of Ps, H_s denotes the interaction term for the static magnetic field, and $H_D(t)$ that for the dynamic (microwave) field which is taken here to be parallel to the x axis;

$$H_D(t)=\tfrac{1}{2}\mu_B g B_d\cos(\omega t)(\sigma_x^{(-)}-\sigma_x^{(+)}) \ .$$

For the choice of the unperturbed states as basis vectors, namely, the triplet states $|\psi_t^0\rangle$, $|\psi_t^1\rangle$, and $|\psi_t^{-1}\rangle$ corresponding to $M=0$, 1, and -1 (see Fig. 2), respectively, and the singlet state $|\psi_s^0\rangle$, we note that the decay matrix λ is diagonal with the elements λ_0 and λ_p. We now proceed to solve (6) by splitting the total Hamiltonian as follows:

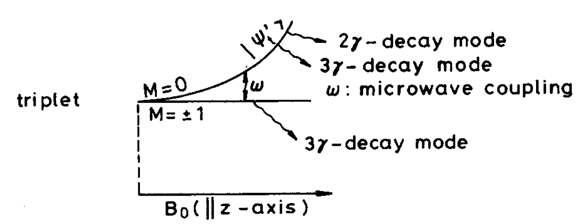

FIG. 2. External microwave-field coupling of the perturbed and unperturbed components of the triplet level. The frequency of the field is ω, strength B_d, and the direction parallel to the x axis.

$$H = H_0 + H'(t) ,$$

where

$$H_0 = H_A + H_s$$

and

$$H'(t) = H_D(t) - \frac{i}{2}\lambda .$$

The basis vectors in which H_0 is diagonal are given by

$$|\psi_t'\rangle = \frac{p}{D}|\psi_t^0\rangle - \frac{\Delta W}{D}|\psi^0\rangle$$

and

$$|\psi_s'\rangle = \frac{\Delta W_s}{D}|\psi_t^0\rangle - \frac{p}{D}|\psi_s^0\rangle$$

together with $|\psi^1\rangle$ and $|\psi_t^{-1}\rangle$, where one defines $D^2 = p^2 + (\Delta W_s)^2$ with

$$\Delta W_s = -\Delta W_t = [p^2 + (\Delta W/2)^2]^{1/2} - \frac{\Delta W}{2} .$$

Expanding $|\psi(t)\rangle$ in terms of these new basis vectors as

$$|\psi(t)\rangle = a_0'(t)|\psi_s'\rangle + a_1'(t)|\psi_t'\rangle + a_1(t)|\psi_t^1\rangle + a_{-1}(t)|\psi_t^1\rangle \tag{8}$$

one obtains the following equations for the amplitudes:

$$i\dot{a}_0' = W_s' a_0' - \frac{i}{2}\Lambda_0 a_0' + \frac{i}{2}\Gamma a_1' - 2V\cos(\omega t)a_+ , \tag{9}$$

$$i\dot{a}_1' = W_t' a_1' - \frac{i}{2}\Lambda_1 a_1' + \frac{i}{2}\Gamma a_0' - 2V\cos(\omega t)a_+ , \tag{10}$$

$$i\dot{a}_+ = W_t a_+ - \frac{i}{2}\lambda_0 a_+ - 4V\cos(\omega t)(a_0' + a_1') , \tag{11}$$

$$i\dot{a}_- = W_t a_- - \frac{i}{2}\lambda_0 a_- , \tag{12}$$

where

$$a_\pm(t) = a_1(t) \pm a_{-1}(t) ,$$

$$V = \frac{x}{4\sqrt{2}}\frac{\Delta W_s}{D}\frac{B_d}{B_0}\Delta W ,$$

$$\Gamma = \frac{p}{D^2}\Delta W_s(\lambda_p - \lambda_0) ,$$

$$\Lambda_0 = \frac{p^2\lambda_p + (\Delta W_s)^2\lambda_0}{D^2} ,$$

and

$$\Lambda_1 = \frac{p^2\lambda_0 + (\Delta W_t)^2\lambda_p}{D^2} .$$

Using

$$\tilde{a}_0' = \exp(iW_s' t)a_0' ,$$

$$\tilde{a}_1' = \exp(iW_t' t)a_1' ,$$

$$\tilde{a}_+ = \exp(iW_t t)a_+ ,$$

and

$$\tilde{a}_- = \exp(iW_t t)a_- ,$$

Eqs. (9)–(12) in the rotating-wave approximation reduce to the following set:

$$i\dot{\tilde{a}}_0' = i\frac{\Gamma}{2}\tilde{a}_1' e^{i(W_s' - W_t')t} - V\tilde{a}_+ e^{i(\omega + W_s' - W_t)t} - i\frac{\Lambda_0}{2}\tilde{a}_0' , \tag{13}$$

$$i\dot{\tilde{a}}_1' = i\frac{\Gamma}{2}\tilde{a}_0' e^{i(W_t' - W_s')t} - V\tilde{a}_+ e^{i(W_t' - W_t - \omega)t} - i\frac{\Lambda_1}{2}\tilde{a}_1' , \tag{14}$$

$$i\dot{\tilde{a}}_+ = -2V(\tilde{a}_0' e^{i(W_t - W_s' - \omega)t} + \tilde{a}_1' e^{i(\omega + W_t - W_t')t}) - i\frac{\lambda_0}{2}\tilde{a}_+ , \tag{15}$$

$$i\dot{\tilde{a}}_- = -i\frac{\lambda_0}{2}\tilde{a}_- . \tag{16}$$

The second and the first term, on the right-hand side of (13) and (15), respectively, rotate even more rapidly than the neglected antirotating terms and have coupling strengths V much weaker than Γ; hence they too are safely neglected.

III. CORRECTION OF THE BREIT-RABI FORMULA

The off-diagonal coupling with respect to Γ in Eqs. (13)–(16), which was neglected in Refs. 6 and 10, are now retained and will be shown to give rise to a small but significant correction to the absorption line-shape function. (We emphasize that the strength Γ is greater by many orders of magnitude than that of the microwave coupling strength V.) Introducing the new amplitudes b_0 and b_1 related by a phase transformation to $\tilde{a}_0'$ and $\tilde{a}_1'$ as

$$b_0 = \tilde{a}_0' e^{-i\phi_0 t}, \quad b_1 = \tilde{a}_1' e^{-i\phi_1 t} ,$$

where

$$\phi_1(\omega) = W_t' - W_t - \omega$$

and

$$\phi_0(\omega) = \phi_1(\omega) + W_s' - W_t'$$

one can reduce the amplitude equations (13)–(15) to the following set:

$$i\dot{b}_0 = \left[\phi_0 - i\frac{\Lambda_0}{2}\right]b_0 + i\frac{\Gamma}{2}b_1 , \tag{17}$$

$$i\dot{b}_1 = i\frac{\Gamma}{2}b_0 + \left[\phi_1 - i\frac{\Lambda_1}{2}\right]b_1 - V\tilde{a}_+ , \tag{18}$$

$$i\dot{\tilde{a}}_+ = -2Vb_1 - i\frac{\lambda_0}{2}\tilde{a}_+ \tag{19}$$

[to shorten writing we omit quoting Eq. (16) from now on].

One can now eliminate the amplitude b_0 by the adiabatic elimination procedure, namely, setting $\dot{b}_0 \simeq 0$ which then, utilizing (17), implies

$$b_0 \simeq -\frac{i}{2}\frac{\Gamma}{\phi_0-\frac{i}{2}\Lambda_0}b_1 . \tag{17a}$$

It may be pointed out in this context that the solution of the amplitude equations are obtained with the assumption that the atom-field interaction begins at a finite initial time, $t=0$. This is consistent with the sudden switching assumption for a constant amplitude microwave field interacting with Ps atoms. This is reasonable for the near resonant terms which satisfy the inequality $t_{\rm rise}<1/\Delta$ where $t_{\rm rise}$ is the actual rise time of the microwave field and Δ is the detuning, but is a poor approximation for the highly off-resonant state for which $t_{\rm rise}>1/\Delta$, since for this state Δ is relatively large (in fact larger than the detuning of the neglected counter-rotating terms).

The adiabatic approximation avoids this inadequacy of the RWA constant amplitude assumption of the microwave field and the consequent sudden switching condition at $t=0$ for all states, by adiabatically eliminating the highly off-resonant terms while retaining explicitly the near-resonant ones.

We set (17a) in (18) to obtain the effective two-level equations:

$$i\dot{b}'_1 = Ve^{i(\phi_1+\Delta)t}\tilde{a}_+ - \frac{i}{2}\Lambda_{1,0}b'_1 , \tag{20}$$

$$i\dot{\tilde{a}}_+ = 2Ve^{i(-\phi_1-\Delta)t}b'_1 - \frac{i}{2}\lambda_0\tilde{a}_+ , \tag{21}$$

where

$$\Delta(\omega)=\frac{1}{4}\frac{\Gamma^2}{\phi_0(\omega)^2+\frac{1}{4}\Lambda_0^2}\phi_0(\omega) , \tag{21a}$$

$$\Lambda_{1,0}(\omega)=\Lambda_1-\frac{1}{4}\frac{\Gamma^2}{\phi_0^2(\omega)+\frac{1}{4}\Lambda_0^2}\Lambda_0 , \tag{21b}$$

and

$$b'_1 = b_1 e^{i[\phi_1(\omega)+\Delta(\omega)]t} .$$

If the terms involving Γ in Eqs. (20) and (21) were neglected, these equations become identical with those used by Theriot *et al.*[6] The error committed by the lowest-order adiabatic approximation can be estimated as follows. We invert Eq. (17) fully to obtain

$$\begin{aligned} b_0(t) &= -\frac{1}{\phi_0-\frac{i}{2}\Lambda_0-i\frac{\partial}{\partial t}}\, i\frac{\Gamma}{2}b_1 \\ &= \frac{-1}{\phi_0-\frac{i}{2}\Lambda_0}\left[1+\frac{1}{\phi_0-\frac{i}{2}\Lambda_0}\left[i\frac{\partial}{\partial t}\right]+\frac{1}{(\phi_0-\frac{i}{2}\Lambda_0)^2}\left[i\frac{\partial}{\partial t}\right]^2+\cdots\right] i\frac{\Gamma}{2}b_1 \\ &= \frac{-i\frac{\Gamma}{2}}{\phi_0-\frac{i}{2}\Lambda_0}b_1+\frac{\frac{\Gamma}{2}}{\left[\phi_0-\frac{i}{2}\Lambda_0\right]^2}\dot{b}_1+\frac{i\frac{\Gamma}{2}}{\left[\phi_0-\frac{i}{2}\Lambda_0\right]^3}\ddot{b}_1+\cdots . \end{aligned}$$

If one now uses (18) to express $\dot{b}_1$ in terms of b_1 one sees immediately that the fractional error in the coefficient of b_1 is of the order 1: $[\phi_1-(i/2)\lambda_1]/[\phi_0-(i/2)\Lambda_0]$ and that of the coefficient of $\tilde{a}_+$ is of the order 1: $i\Gamma/2/[\phi_0-(i/2)\Lambda_0]$. These errors are therefore certainly less than 1: $O(\omega_r/\Delta W)$ where ω_r is the resonance frequency.

Equations (20) and (21) can be solved directly to obtain the 2γ signal for the microwave resonance absorption. Denoting by $\Lambda_{2\gamma}$ the 2γ component of the decay rate of the perturbed triplet state, we take the usual definition of the 2γ decay probability as given by

$$P_{0,0}=\Lambda_{2\gamma}\int_0^\infty |b'_1(t)|^2dt,\quad P_{1,0}=P_{-1,0}=\Lambda_{2\gamma}\int_0^\infty |b'_1(t)|^2dt ,$$

where for $P_{0,0}$ the amplitude $b'_1(t)$ is calculated with the initial conditions $a'_1(0)=1$ and $a_1(0)=a_{-1}(0)=0$; for $P_{1,0}$ one uses the initial conditions $a'_1(0)=a_{-1}(0)=0$ and $a_1(0)=1$; and finally for $P_{-1,0}$ one sets the initial conditions $a_{-1}(0)=1$ and $a'_1(0)=a_1(0)=0$. One thereby gets, after simplifying the algebra, the following result:

$$P_{0,0}=\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}}\frac{2|V|^2(\Lambda_{1,0}+\lambda_0)/\lambda_0+\frac{1}{4}(\Lambda_{1,0}+\lambda_0)^2+(\phi_1+\Delta)^2}{(\phi_1+\Delta)^2+\frac{1}{4}(\Lambda_{1,0}+\lambda_0)^2\left[1+\frac{8|V|^2}{\Lambda_{1,0}\lambda_0}\right]} , \tag{22}$$

$$P_{1,0}=\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}}\frac{|V|^2(\Lambda_{1,0}+\lambda_0)/\lambda_0}{(\phi_1+\Delta)^2+\frac{1}{4}(\Lambda_{1,0}+\lambda_0)^2\left[1+\frac{8|V|^2}{\Lambda_{1,0}\lambda_0}\right]} . \tag{23}$$

The total 2γ signal, after subtracting the background $\Sigma_{2\gamma}(\omega)$, is then given by

$$\Sigma_{2\gamma}(\omega)=\tfrac{1}{4}\left[P_{1,0}+P_{-1,0}+P_{0,0}-\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}}\right] \tag{24a}$$

$$=\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}(\omega)}\frac{\Lambda_{1,0}^2(\omega)-\lambda_0^2}{2\Lambda_{1,0}(\omega)\lambda_0}\frac{|V|^2}{[\phi_1(\omega)+\Delta(\omega)]^2+\frac{1}{4}[\Lambda_{1,0}(\omega)+\lambda_0]^2\left[1+\dfrac{8|V|^2}{\Lambda_{1,0}(\omega)\lambda_0}\right]} . \tag{24b}$$

Equation (24) is the desired line-shape function which corrects the usual Breit-Rabi formula.

Before proceeding further it is worthwhile to draw the reader's attention to a number of inconsistencies, presumably due to the existence of misprints in the earlier literature. The standard work of Theriot *et al.*[10] provided the definitions and derived the line-shape functions (prior to the need for inclusion of the off-diagonal coupling terms due to the annihilation, onto the line shape) which have been followed by most authors subsequently. In that paper the line shape to fit the data is defined as

$$P_T=\tfrac{1}{2}\left[P_{1,0}+P_{-1,0}+\left[P_{0,0}-\frac{\lambda_{10,2}}{\lambda_{1,0}}\right]\right] \tag{25}$$

[see Eq. (20) there] where the probability $P_{M,0}$ is the probability that the atom decays by 2γ annihilation from the perturbed (in the BR representation) magnetic state $M=\pm 1,0$. Furthermore $\lambda_{10,2}$ is the 2γ component of the total decay rate $\lambda_{1,0}$ of the triplet state $M=0$ [see Eq. (7a) there]. In the subsequent work Egan *et al.*[5] used the method of Theriot *et al.*[10] to calculate the decay signal as

$$S=\frac{\lambda_{10,2}}{4\lambda_{1,0}}+\left[\frac{\lambda_{10,2}}{\lambda_{1,0}}(\lambda_0+\lambda_{1,0})\frac{V^2}{\hbar^2}\left[\frac{1}{2\lambda_0}-\frac{1}{\lambda_{1,0}}\right]\left[\frac{1}{(\omega-\omega_{01})^2+\frac{1}{2}(\lambda_0+\lambda_{1,0})+2(\lambda_0+\lambda_{1,0})^2V^2/\lambda_{1,0}\lambda_0\hbar^2}\right]\right] .$$

In an attempt to rederive the above formula we found that the definition of S [e.g., Eq. (5) of Egan *et al.*[5]] is not consistent with the definition of P_T above [i.e., Eq. (20) of Theriot *et al.*[10]] but to the following definition:

$$P_T'=\frac{\lambda_{10,2}}{4\lambda_{1,0}}+\frac{1}{4}\left[P_{1,0}+P_{-1,0}+2\left[P_{0,0}-\frac{\lambda_{10,2}}{\lambda_{1,0}}\right]\right] . \tag{26}$$

Note particularly the difference in the factor of 2 before the third term in the second set of large parentheses and in the large square brackets of Eq. (25) and Eq. (26). (In formula (5) of Egan *et al.*[5] there is an obvious printing error missing the square sign from the term $[\frac{1}{2}(\lambda_0+\lambda_{1,0})]^2$ in the denominator. This printing error has been corrected by Rich[1] in his review and by Mills[8] who also adds a $\frac{1}{4}$ to the formula of the signal while quoting this formula, but the difference in the weighting factors remained unnoticed.) Equation (26) leads to an unequal weighting of the $P_{0,0}$ probability with respect to $P_{1,0}$ or $P_{-1,0}$ probabilities while Eq. (25) maintains an equal weighting factor of $P_{0,0}$ with respect to $P_{1,0}$ and $P_{-1,0}$. This factor also arises in the older paper of Hughes *et al.*,[6] where it has been introduced on the ground of "separate consideration of transitions between $M=0$ and $+1$ and between $M=0$ and -1 orthopositronium states in the approximation applicable to low microwave fields that the coupling of the three states can be neglected."

We may also note that the expression for P_T above [Eq. (20) in Theriot *et al.*[10]] reduces for small values of x to their Eq. (22a) multiplied by the factor $[\frac{1}{2}x^2(\lambda_p/\lambda_0)]$.

In the limit $\Gamma\to 0$ Eq. (24) goes over to

$$\Sigma_{2\gamma}(\omega)=\frac{\lambda_{10,2}}{\lambda_{1,0}}\frac{\lambda_{1,0}^2-\lambda_0^2}{2\lambda_{1,0}\lambda_0}\frac{|V|^2}{(\omega_{01}-\omega)^2+\left[\dfrac{\lambda_{1,0}+\lambda_0}{2}\right]^2\left[1+\dfrac{8|V|^2}{\lambda_{1,0}\lambda_0}\right]} . \tag{27}$$

If, however, the signal is defined as [cf. Hughes *et al.*,[6] Eq. (30)]

$$\Sigma_{2\gamma}'(\omega)=\frac{\Lambda_{2\gamma}}{4\Lambda_{1,0}(\omega)}+\frac{1}{4}\left[P_{1,0}+P_{-1,0}+2\left[P_{0,0}-\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}(\omega)}\right]\right] , \tag{28}$$

we get

$$\Sigma_{2\gamma}'(\omega)=\frac{\Lambda_{2\gamma}}{4\Lambda_{1,0}(\omega)}+\frac{\Lambda_{2\gamma}}{\Lambda_{1,0}(\omega)}(\Lambda_{1,0}+\gamma_0)\left[\frac{1}{2\lambda_0}-\frac{1}{\Lambda_{1,0}(\omega)}\right]\frac{|V|^2}{[\phi_1(\omega)+\Delta(\omega)]^2+\frac{1}{4}[\Lambda_{1,0}(\omega)+\lambda_0]^2\left[1+\dfrac{8|V|^2}{\Lambda_{1,0}(\omega)\lambda_0}\right]} . \tag{29}$$

This will, in the limit $\Gamma \to 0$, go over to the result of Egan *et al.*,[5] namely,

$$\Sigma'_{2\gamma}(\omega)=\frac{\lambda_{10,2}}{4\lambda_{1,0}}+\left[\frac{\lambda_{10,2}}{\lambda_{1,0}}(\lambda_0+\lambda_{1,0})\left[\frac{1}{2\lambda_0}-\frac{1}{\lambda_{1,0}}\right]\frac{|V|^2}{\left[(\omega-\omega_{01})^2+\left[\frac{\lambda_{1,0}+\lambda_0}{2}\right]^2+\frac{2(\lambda_{1,0}+\lambda_0)^2|V|^2}{\lambda_{1,0}\lambda_0}\right]}\right]. \qquad (30)$$

In the further discussions below we shall restrict ourselves to the definition as in (24a) and the signal $\Sigma_{2\gamma}$, Eq. (24b), rather than (28) and the corresponding signal, (29), $\Sigma_{2\gamma}$.

IV. DISCUSSIONS

One sees immediately that the 2γ signal, $\Sigma_{2\gamma}$ [Eq. (24b)], is a slightly asymmetric spectrum because of the dependence of the width $\Lambda_{1,0}(\omega)$ on ω (see Fig. 3). An asymmetric line shape in the present context has been found first by Mills[8] in an alternative way. It is interesting to note that if this ω dependence is neglected then the line shape becomes symmetric and the line center coincides with the zero of $\phi_1(\omega)+\Delta(\omega)=0$. This leads to

$$\frac{\Delta W-\Delta W_0}{\Delta W}=q^2\frac{1}{2}\left[1+\frac{1}{(1+x^2)^{1/2}}\right]\times\left[1+x^2+\left[\frac{\lambda_p}{2\Delta W}\right]^2\right]^{-1}, \qquad (31)$$

where, as before, $q=(\lambda_p-\lambda_0)/(2\Delta W)$ and $\Delta W_0=2\omega/(1+x^2)^{1/2}+1$.

Formula (27) agrees with that obtained by Rich[7] using his heuristic method [cf. Eq. (5)], when one neglects the term $(\lambda_p/2\Delta W)^2 \simeq 3.9\times10^{-4}$ compared to $x^2 \simeq 4.8\times10^{-2}$.

Rich has already used[7] this formula to adjust the experimental ΔW values previously reported. However, we note that the derivation given above of (27) clearly requires the neglect of the ω dependence of $\Lambda_{1,0}(\omega)$ and $\Delta(\omega)$, which also make the otherwise slightly asymmetric line shape symmetric. One may expect that the neglect of the ω dependence of $\Lambda_{1,0}(\omega)$ and the formula (27) could be reasonable. However, Mills[8] has pointed out that the experiments are sensitive to the line-shape asymmetry because the line center is determined mostly from data points where the slope of the resonance is the largest. This indicates that it would be perhaps more appropriate to use directly the full line-shape function (24b) to provide *ab initio* analysis of future experimental data.

It is difficult to compare the numerical method of Mills who worked in the unperturbed representation with our analytical method in the BR representation. In so far as the Hamiltonians used in the two representations are the same, the result obtained using the same initial condition should of course be identical. However, we note that after the representations have been chosen, Mills[8] and we make further approximations [Mills neglects the small z terms in his Eq. (9), while we make the adiabatic elimination approximation] which lead to solutions which are no longer exact (with respect to the original Hamiltonian) and then also are not completely equivalent.

Below, we show the signal as given by $\Sigma_{2\gamma}(\omega)$ [Eq. (24b)] as a function of x in Fig. 4. For the purpose of illustration we have set (cf. Mills[8]): $y=2\times10^{-5}$ and $\omega=3.25$ GHz (with $\Delta W=203.385$ GHz, $\lambda_0=\frac{1}{142}$ GHz, and $\lambda_p=8$ GHz). For the same parameter values the peak for Mills's computation is

$$x_{\text{peak}}=2x_p=2\times0.127\,415\,955\,1\ ,$$

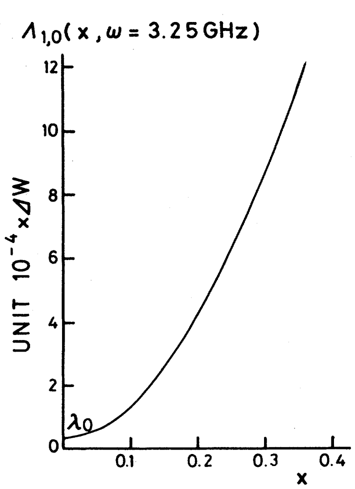

FIG. 3. "Effective" decay constant $\Lambda_{1,0}(\omega)$ as a function of the parameter x plotted in units of $10^{-4}\times$ hyperfine separation.

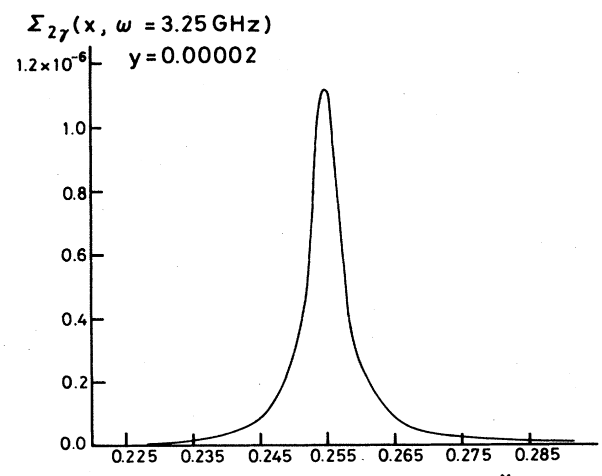

FIG. 4. Signal as given by Eq. (24b) plotted for microwave frequency $w=3.25$ GHz and $y=(B_d/2\sqrt{2})(g\mu_B/\Delta w)=2\times10^{-5}$.

whereas we find the peak of the line shape (24b) at

$$x_{\text{peak}} = 0.254\,884\,555\,1\ .$$

Although these two values are very close, there exists the difference at the fifth decimal place. On the other hand, we note that the height of Mill's line shape differs by several orders of magnitude from our result. In the absence of an analytical result in Mills's work it is difficult to see where exactly this difference comes from. We note, however, that for small values of x our signal is of the same order of magnitude as that given by the usual Breit-Rabi formula [see Theriot *et al.*,[10] Eq. (22a) for P_T].

ACKNOWLEDGMENTS

We would like to thank Professor A. Rich for stimulating our interest in this problem during his visit to the University of Bielefeld. We are also indebted to Dr. A. P. Mills for mailing his works on the subject to us prior to publication. This work was supported by the Universität Bielefeld Research Project No. OZ2891.

[1]A. Rich, Rev. Mod. Phys. **53**, 127 (1981).
[2]D. W. Gidley, Can. J. Phys. **60**, 543 (1982).
[3]G. Lepage, in *Proceedings of the 7th International Conference on Atómic and Molecule Physics, Cambridge, August, 1980,* edited by D. Kleppner and F. M. Pipkin (Plenum, New York, 1981), p. 297.
[4]M. Deutsch and S. C. Brown, Phys. Rev. **85**, 1047 (1952).
[5]P. O. Egan, V. W. Hughes, and M. H. Yam, Phys. Rev. A **15**, 251 (1977).
[6]V. W. Hughes, S. Marder, and C. S. Wu, Phys. Rev. **106**, 934 (1957).
[7]A. Rich, Phys. Rev. A **23**, 2747 (1981). (This is the paper referred to in the abstract.)
[8]A. P. Mills, Jr., Phys. Rev. A **27**, 262 (1983).
[9]O. Halpern, Phys. Rev. **94**, 904 (1954).
[10]E. D. Theriot, Jr., R. H. Beers, V. W. Hughes, and K. O. H. Ziock, Phys. Rev. A **2**, 707 (1970).
[11]A. P. Mills, Jr. and G. H. Bearman, Phys. Rev. Lett. **34**, 246 (1975).
[12]E. R. Carlson, V. W. Hughes, and I. Lindgren, Phys. Rev. A **15**, 241 (1977).
[13]A. P. Mills, Jr., J. Chem. Phys. **62**, 2646 (1975).