Vector Potential Versus Field Intensity

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This paper deals with the apparent breakdown of gauge invariance in atomic-level-width formulas. Specifically, it is shown that in the analysis of the measurement od the Lamb shift the use of the $\vec{p}\cdot\vec{A}/(mc)$ and the $\vec{E}\cdot\vec{r}$ forms of the interaction yields almost identical results for the shape of the resonance curve and equal positions for the line center. This is achieved by adding the contribution of all intermediate states to the basic three-level resonance formula. While the contribution of these intermediate states in the $\vec{E}\cdot\vec{r}$ language is negligible, it is nevertheless significant when the $\vec{p}\cdot\vec{A}(mc)$ form of the interaction is used. Although this particular example would indicate that the use of the $\vec{E}\cdot\vec{r}$ form of the interaction is computationally simpler, it is shown that no general statement to this effect is permissible. A simple counter example is presented within the context of elastic photon scattering off atomic targets.

I. INTRODUCTION

Although the existence of a gauge transformation which eliminates the $\vec{p}\cdot\vec{A}/mc$ and the $\vec{A}\cdot\vec{A}/2mc^2$ terms from the nonrelativistic Hamiltonian and replaces them by $\vec{E}\cdot\vec{r}$ has been known for a long time,[1] the only systematic study of this question known to this author is the work of Power and Zienau.[2] These authors claim that whenever a discrepancy arises between matrix elements obtained by the use of the two forms of the electric-dipole interaction, the result obtained with the $\vec{E}\cdot\vec{r}$ form is the correct one. This is difficult to understand, since the physical results expressed by these matrix elements are expected to be gauge invariant.

A more baffling question is posed by the long-standing observation of Lamb[3] that the use of the $\vec{p}\cdot\vec{A}/mc$ form of the electric-dipole interaction in the Bethe-Lamb formula yields a line shape in disagreement with experiment. The aim of this work is to clarify these questions and to delineate the conditions under which matrix elements computed with the two differing forms of the electric-dipole interaction are identical. To put things in their proper perspective, it is necessary to distinguish between two types of matrix elements. The first category consists of matrix elements in which radiation damping does not appear. These matrix elements can be obtained within the context of perturbation expansions, starting with semiclassical radiation theory. The second group consists of matrix elements involving radiation damping, such as level-width formulas. Although the gauge invariance for several examples belonging to the first category, such as the Heisenberg-Kramers dispersion formula[1] and the double quantum decay of the $2S$ level of hydrogen,[4] was already demonstrated in the literature, I shall nevertheless give another illustration: to wit, the lowest-order nonvanishing matrix element for bremsstrahlung by a neutral particle off a neutral atom.

The example to be treated here will serve to underline the conditions under which equivalence is obtained in practical calculations. These requirements are (i) that the physical process described by the matrix element conserve energy, and (ii) that to a given order in the radiation field all coherent processes must be included. This example will be presented in Sec. II. Having learned from these examples that even for matrix elements of the first category equivalence can be obtained only when the above conditions are fulfilled, we apply these ideas to remove discrepancies in level-width formulas obtained via the two forms of the interaction. In Sec. III we discuss as an example of the second-category matrix element the quenching of the $2S$ level of hydrogen by an external frequency-tunable microwave field. The microwave frequency is in the vicinity of the Lamb separation. We find that including all intermediate states with the basic Bethe-Lamb formula, when use is made of the vector potential, removes a large part of the discrepancy. In Sec. IV we address ourselves to the more realistic case—the one encountered in the measurement of the Lamb shift. We discuss the quenching of the $2S$ state of hydrogen in the simultaneous presence of external fixed-frequency microwave field and a (tunable) dc magnetic field. If we insert the vector potential into the basic Bethe-Lamb expression, we find that the contributions from the rest of the intermediate P states cannot be ignored. Including them removes the major discrepancy between the vector potential and field-intensity formulation of

the problem. Fortuitously, in the presence of a (tunable) dc magnetic field the position of the line center is now identical. There remains a small discrepancy between the two (symmetric) line shapes. Plausible reasons for this are advanced, among which is the observation that adding on the background terms without modifying the original Bethe-Lamb formula is an *ad hoc* procedure.

Although in opting for the $\vec{E}\cdot\vec{r}$ form of the electric-dipole interaction the Bethe-Lamb formula remains much simpler, inasmuch as only a finite number of levels have to be considered, unlike in the $\vec{p}\cdot\vec{A}/mc$ form of the interaction where all levels have to be included, one cannot conclude from this that the field-intensity formulation is generally superior to that of the vector potential. In Sec. V we present a simple counterexample to this proposition. We approximate the Kramers-Heisenberg dispersion formula for hydrogen in the vicinity of a resonance (but far enough from the center of the resonance so that the damping term can be dropped) by neglecting all but the nearest intermediate level. Here the $\vec{E}\cdot\vec{r}$ form of the interaction is second best. The numbers are compared with the exact result obtained by Gavrila.[5] Finally, our conclusions are summarized in Sec. VI.

II. GAUGE TRANSFORMATION AND EQUIVALENCE OF MATRIX ELEMENTS WITHOUT RADIATION DAMPING

The nonrelativistic Schrödinger equation for the one-particle Coulomb problem, including the vector potential, is

$$\left(\frac{[\vec{p}+(e/c)\vec{A}]^2}{2m}-\frac{e^2}{r}\right)\psi=i\hbar\frac{\partial\psi}{\partial t}, \tag{1}$$

where the notation has its usual meaning. It is well known[1,2] that the above equation can be transformed by a unitary operator, which eliminates the vector potential in favor of the electromagnetic field intensity. For the special case when only the electric-dipole interaction enters into consideration, as in our subsequent discussion, the unitary operator is given by

$$U=\exp[+ie\vec{r}\cdot\vec{A}(t)/\hbar c]. \tag{2}$$

The transformed Hamiltonian H' is obtained from the following expression:

$$\psi'\left[U\left(H-i\hbar\frac{\partial}{\partial t}\right)U^{-1}\right]=H'\psi'. \tag{3}$$

Thus

$$H'=P^2/2m-e^2/r+e\vec{E}(t)\cdot\vec{r}, \tag{4}$$

where

$$\vec{E}=-\left(\frac{1}{c}\right)\frac{\partial\vec{A}}{\partial t}. \tag{5}$$

Writing H and H' as a sum of H_0+H_I, and $H_0'+H_I'$, we see that H_0 and H_0' are formally identical and

$$H_I=(e/mc)\vec{A}\cdot\vec{p}+e^2A^2/2mc^2, \tag{6}$$

while

$$H_I'=e\vec{E}\cdot\vec{r}. \tag{7}$$

Obviously the inner product of any two time-dependent solutions of Eq. (1) will be equal to the inner product of the corresponding solutions of Eq. (3). The problem at hand is, however, different since we are compelled to work within the context of perturbation theory. And while there is no *a priori* reason why perturbation theory should fail for these problems, it is nevertheless the case that H_0' is not the unitary transform of H_0. So the central question remains—namely, under what conditions are the two forms of the perturbation expansion identical? Clearly, one should be able to supply the answer by mathematical reasoning.[6] Here, however, we shall merely state the conditions without a general proof. Matrix elements of H_I are identical with those obtained from H_I' in any order of the expansion provided that (i) over-all energy is conserved and (ii) that to a given order in the expansion all coherent terms are included. We are led to this generalization partly by the detailed examples in atomic physics[1,4] and also by analogy with relativistic electrodynamics. Recall that in quantum electrodynamics the perturbation-theoretic amplitudes are invariant under a gauge transformation only if (i) four momentum is conserved and (ii) all the coherent terms to a given order in the expansion are included.[7] Consider, for example, the matrix element of photon emission (absorption) between two states of the hydrogen atom:

$$M(t=0)=(e/mc)\langle\psi_i|\vec{A}\cdot\vec{p}|\psi_f\rangle \tag{8}$$

and

$$M'(t=0)=e\langle\psi_i'|\vec{E}\cdot\vec{r}|\psi_f'\rangle. \tag{8a}$$

Since $\vec{p}/m=(i/\hbar)[H_0,\vec{r}]$, the above can be written as

$$M=(16\pi^3\hbar\omega)^{-1/2}\,i(E_i-E_f)\langle\psi_i|\vec{\epsilon}\cdot\vec{r}|\psi_f\rangle \tag{9}$$

and

$$M'=(16\pi^3\hbar\omega)^{-1/2}\,(\pm i\hbar\omega)\langle\psi_i'|\vec{\epsilon}\cdot\vec{r}|\psi_f'\rangle, \tag{9a}$$

where E_i, E_f, ω, and $\vec{\epsilon}$ have their customary meaning. In view of the circumstance that H_0 is formally identical with H_0', the superscripts on ψ_i' and ψ_f' can be dropped. It is immediately obvious that M and M' are equal only if $E_i-E_f=\hbar\omega$.

When energy is not conserved, the matrix element does not represent a physical process. Such a matrix element can appear, however, as part of a more complex expression in which over-all energy is conserved. A concrete example is bremsstrahlung by a neutral particle incident on atomic hydrogen. The reaction can be characterized as

$$\vec{q}+a\rightarrow\vec{q}'+a+\hbar\vec{k}. \tag{10}$$

Here $\vec{q}$ and $\vec{q}'$ denote the initial and final momentum of the projectile, $\hbar\vec{k}$ stands for the momentum of the emitted photon, and a stands for the atomic ground state. The matrix element for the above reaction in the Born approximation is

$$T=\sum_n\frac{\langle i|O_1|n\rangle\langle n|O_2|f\rangle}{E_i-E_n}+\sum_m\frac{\langle i|O_2|m\rangle\langle m|O_1|f\rangle}{E_i-E_m}, \tag{11}$$

where

$$|i\rangle=|\vec{q},a\rangle,\quad |f\rangle=|\vec{q}',a\rangle,$$
$$|n\rangle=|\vec{q}',a_n\rangle,\quad |m\rangle=|\vec{q},a_m\rangle,$$

and

$$E_i=\hbar^2q^2/2m+\epsilon_0,\quad E_n=\hbar^2(q')^2/2m+\epsilon_n,$$
$$E_m=\hbar\omega+\epsilon_m+\hbar^2q^2/2m.$$

The operator O_1 is some unspecified function of the position coordinates only, and

$$O_2=(e/mc)\vec{A}\cdot\vec{p}. \tag{12}$$

a_n stands for the nth excited atomic level (discrete and continuum) and ϵ_n is the corresponding energy. We now proceed to show that Eq. (11) is invariant under the interchange of O_2 with $e\vec{E}\cdot\vec{r}$. Since

$$\langle i|O_2|m\rangle=(ie/\hbar c)\epsilon_{0,m}\langle i|\vec{A}\cdot\vec{r}|m\rangle \tag{13}$$

and

$$\langle n|O_2|f\rangle=(ie/\hbar c)\epsilon_{n,0}\langle n|\vec{A}\cdot\vec{r}|f\rangle, \tag{14}$$

where

$$\epsilon_{0,m}=\epsilon_0-\epsilon_m, \tag{15}$$

it follows that Eq. (11) can be written as

$$T=\left(\frac{ie}{\hbar c}\right)\sum_n\frac{\langle i|O_1|n\rangle\langle n|\vec{A}\cdot\vec{r}|f\rangle\epsilon_{n,0}}{E_i-E_n}+\left(\frac{ie}{\hbar c}\right)\sum_m\frac{\langle i|\vec{A}\cdot\vec{r}|m\rangle\langle m|O_1|f\rangle\epsilon_{0,m}}{E_i-E_m}. \tag{16}$$

Exploiting energy conservation $(\hbar^2/2m)[q^2-(q')^2]=\hbar\omega$, the above can be cast in the form

$$T=\left(\frac{ie\omega}{c}\right)\sum_n\frac{\langle i|O_1|n\rangle\langle n|\vec{A}\cdot\vec{r}|f\rangle}{E_i-E_n}+\left(\frac{ie\omega}{c}\right)\sum_m\frac{\langle i|\vec{A}\cdot\vec{r}|m\rangle\langle m|O_1|f\rangle}{E_i-E_m}-\left(\frac{ie}{\hbar c}\right)\sum_n\langle i|O_1|n\rangle\langle n|\vec{A}\cdot\vec{r}|f\rangle$$
$$+\left(\frac{ie}{\hbar c}\right)\sum_m\langle i|\vec{A}\cdot\vec{r}|m\rangle\langle m|O_1|f\rangle. \tag{17}$$

Completeness of the atomic states and the circumstance that $\vec{A}\cdot\vec{r}$ and O_1 commute ensure the vanishing of the last two terms. The remaining terms are precisely the ones obtained with the $e\vec{E}\cdot\vec{r}$ form of the electric-dipole interaction. Other examples can be found in the literature: the Kramers-Heisenberg dispersion formula[1] and the two-photon decay of the metastable 2S level of hydrogen.[4] The essential points to be learned from these examples are (i) that equivalence is only obtained for matrix elements which are energy conserving, and (ii) that all intermediate states which contribute coherently have to be included. We now proceed to apply these considerations to matrix elements with radiation damping.

III. MATRIX ELEMENTS WITH RADIATION DAMPING

A striking example of the apparent breakdown of the equivalence between the $\vec{p}\cdot\vec{A}/mc$ and the $\vec{E}\cdot\vec{r}$ forms of the electric-dipole interaction is found in the Bethe-Lamb formula. This expression gives the shape of the level width for the decay of the metastable $2\,^2S_{1/2}$ level of hydrogen in the presence of a quenching field. It is the formula used to extract the Lamb shift from the measured level width. In particular, when the quenching is via a microwave field, as in the classical version of this experiment,[3] the use of the vector potential in the Bethe-Lamb formula yields a line shape in contradiction with the observed data. Our discussion is addressed to this problem.

Although in the actual experiment the frequency of the microwave field is kept fixed and the line shape is obtained by tuning the various magnetic sublevels of the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ levels with a dc magnetic field, we first analyze the problem without a magnetic field. To obtain a level width we allow for a tunable microwave field. Since this is a "gedanken" experiment we can ignore the practical difficulty involved with frequency tuning. And to simplify things a bit more we omit the spin of the electron. We assume that the Lamb shift is

accounted for by including a phenomenological term in the Hamiltonian which removes the degeneracy between the 2S and 2P levels. Our Hamiltonian, including the (semiclassical) vector potential, is

$$\left(\frac{[\vec{p}+(e/c)\vec{A}]^2}{2m}-\frac{e^2}{r}+8\pi\kappa a_0^3\delta^{(3)}(\vec{r})\right)\psi=i\hbar\frac{\partial\psi}{\partial t}, \tag{18}$$

where a_0 is the radius of the lowest Bohr orbit and κ is the Lamb energy.[8] Applying the unitary transformation of Eqs. (2) and (3) to (18), we obtain

$$H'=P^2/2m-e^2/r+8\pi\kappa a_0^3\delta^{(3)}(\vec{r})+e\vec{r}\cdot\vec{E}(t). \tag{19}$$

The transition amplitude for the decay of the 2S state in the presence of a (weak) external microwave field is

$$T=\frac{\langle 2S|O(1)|2P\rangle\langle 2P|O(2)|1S\rangle}{\kappa-\hbar\omega_1+\frac{1}{2}i\Gamma}+\sum_{n\neq 2}\frac{\langle i|O(1)|n\rangle\langle n|O(2)|f\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_1}+\sum_n\frac{\langle i|O(2)|n\rangle\langle n|O(1)|f\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_2}, \tag{20}$$

where $|i\rangle=|2S\rangle$, $|f\rangle=|1S\rangle$, and it is tacitly assumed that the initial 2S wave function includes the correction (at least to first order) due to the phenomenological $8\pi\kappa a_0\delta^{(3)}(\vec{r})$ term. $O(1)=e\vec{p}\cdot\vec{A}_1/mc$ and $O(2)=e\vec{p}\cdot\vec{A}_2/mc$. The intermediate states all have angular momentum one. Using the $\vec{E}\cdot\vec{r}$ form of the interaction, one obtains a similar result:

$$T'=\frac{e^2\langle i|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|f\rangle}{\kappa-\hbar\omega_1+\frac{1}{2}i\Gamma}+\sum_{n\neq 2}\frac{e^2\langle i|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|f\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_1}+\sum_n\frac{e^2\langle i|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|f\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_2}. \tag{21}$$

We now write

$$T=R+B \tag{22}$$

and

$$T'=R'+B', \tag{23}$$

where R and R' denote the resonant parts of T and T', respectively. The apparent breakdown of the unitary transformation is most conspicuous, as was first observed by Lamb,[3] when one compares R with R'. Using Eq. (14) we can rewrite R as follows:

$$R=\frac{-e^2\kappa\epsilon_{2,1}\langle i|\vec{A}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{A}_2\cdot\vec{r}|f\rangle}{(\hbar c)^2(\kappa-\hbar\omega_1+\frac{1}{2}i\Gamma)}, \tag{24}$$

$$R'=\frac{-e^2\omega_1\omega_2\langle i|\vec{A}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{A}_2\cdot\vec{r}|f\rangle}{\kappa-\hbar\omega_1+\frac{1}{2}i\Gamma}, \tag{25}$$

where ω_1 and ω_2 are the angular frequencies of the microwave and Lyman-α photons, respectively. The corresponding transition probabilities are proportional to:

$$W=\frac{e^4\kappa^2(E_2-E_1)^2|M|^2\omega_2}{\omega_1(\hbar c)^4[(\kappa-\hbar\omega_1)^2+\frac{1}{4}\Gamma^2]} \tag{26}$$

and

$$W'=\frac{e^4\omega_1\omega_2^3|M|^2}{(\kappa-\hbar\omega_1)^2+\frac{1}{4}\Gamma^2}. \tag{27}$$

The common factor $|M|^2$ is defined as

$$|M|^2=\omega_1\omega_2|\langle i|\vec{A}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{A}_2\cdot\vec{r}|f\rangle|^2. \tag{28}$$

Equations (26) and (27) differ from each other both in the line shape and in the position of the maximum. Introducing dimensionless variables, $x=(\kappa-\hbar\omega_1)/\kappa$ and $\Gamma/\kappa=\lambda$, the right-hand side of Eq. (26) is proportional to

$$[(1-x)(x^2+\tfrac{1}{4}\lambda^2)]^{-1}, \tag{29}$$

while the r.h.s. of Eq. (27) is proportional to

$$(1-x)/(x^2+\tfrac{1}{4}\lambda^2). \tag{30}$$

Since the change in ω_2 due to variations in ω_1 is negligible, the apparent maximum of Eq. (26) is at $x=\frac{1}{8}\lambda^2$, while the maximum of Eq. (27) is at $x=-\frac{1}{8}\lambda^2$. Using the physical values for the Lamb shift and the lifetime of the 2P state, it follows that the two maxima are displaced from each other by $\frac{1}{4}\lambda^2$. This large discrepancy can be removed, however, if, as indicated before, we recognize that the unitary transformation which connects the two forms of the electric dipole-interaction (at least in the semiclassical theory) can, at best, yield identical results only if we include all the coherent terms in the amplitude. We now proceed to show this by computing B and B' (the background terms) and adding them to the resonant parts of the amplitude.

To simplify things we now make the following approximations. All states appearing in B and B' are assumed to be eigenstates of the Coulomb Hamiltonian without the phenomenological Lamb term. B and B' can be easily evaluated using methods pioneered by Dalgarno and Lewis.[9] Since we are mainly interested in a region of ω_1 close to the resonance frequency, where $\omega_1/\omega_2\ll 1$, further simplifications are possible. Our starting point is the following identity:

$$e^2\sum_n \frac{\langle 2S|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_1}+e^2\sum_n \frac{\langle 2S|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_2}$$
$$=\sum_n \frac{\langle 2S|O(1)|n\rangle\langle n|O(2)|1S\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_1}+\sum_n \frac{\langle 2S|O(2)|n\rangle\langle n|O(1)|1S\rangle}{\epsilon_2-\epsilon_n-\hbar\omega_2}. \quad (31)$$

This identity, which follows from the unitary transformation given in Eq. (2), is proved in Ref. 4 and also in the Appendix, subject, of course, to the conditions stated earlier: that energy be conserved, i.e., $\epsilon_2-\epsilon_1=\hbar(\omega_1+\omega_2)$, and that the summation is over a complete set of states. It is important to notice that on the left-hand side (l.h.s.) of the above equation the $2P$ intermediate state adds a finite contribution to the sum, while on the r.h.s. the matrix element involving the $2P$ level is zero. This follows from the use of the dipole approximation and the degeneracy of the unperturbed $2S$ and $2P$ levels. Thus, to zeroth order in the Lamb operator, B is identical with the r.h.s. of Eq. (31), while B' differs from the l.h.s. of (31) by the omission of the $2P$ state in the first sum of Eq. (21). Combining Eqs. (20), (21), and (31) we find that, to zeroth order in the Lamb operator,

$$B=B'+\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{-\hbar\omega_1}. \quad (32)$$

Since B' is of the order ω_1/ω_2 (see Appendix), we can approximate T and T' in the following fashion:

$$T=R-\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{\hbar\omega_1} \quad (33)$$

and

$$T'=R'. \quad (34)$$

The new approximate transition probabilities are now proportional to

$$W\propto\frac{1-2x+x^2+\frac{1}{4}\lambda^2}{(1-x)(x^2+\frac{1}{4}\lambda^2)} \quad (35)$$

and

$$W'\propto\frac{(1-x)}{x^2+\frac{1}{4}\lambda^2}. \quad (36)$$

Although (35) and (36) are not quite identical, the difference in the position of the two maxima is reduced considerably. $x_0-x_0'=-\frac{1}{16}\lambda^4$. Plausible reasons for the remaining disagreement will be given at the end of Sec. IV, where we discuss the question of the equivalence of the two forms of the interaction operator in the presence of a dc magnetic field.

IV. EXTENSION TO MAGNETIC FIELD TUNING

Having demonstrated that for matrix elements without radiation damping the two forms of the electric-dipole interaction yield identical results, and that with radiation damping almost identical results are obtained, we not proceed to show that the introduction of a weak external magnetic field leads to conclusions similar to the ones obtained in Sec. III. The phenomenological Hamiltonian, to first order in the external magnetic field, is

$$\left(\frac{[\vec{p}+(e/c)\vec{A}]^2}{2m}-\frac{e^2}{r}+\frac{e\vec{\mathcal{H}}\cdot\vec{L}}{2mc}+8\pi\kappa a_0^3\delta^{(3)}(\vec{r})+\frac{e^2}{2mc^2}\vec{A}\cdot(\vec{\mathcal{H}}\times\vec{r})\right)\psi=i\hbar\frac{\partial\psi}{\partial t}. \quad (37)$$

Applying the unitary transformation of Eqs. (2) and (3) to (37), we obtain

$$H'=p^2/2m-e^2/r+8\pi\kappa a_0^3\delta^{(3)}(\vec{r})+e\vec{\mathcal{H}}\cdot\vec{L}/2mc+e\vec{r}\cdot\vec{E}. \quad (38)$$

It is worth noting that in the presence of an external magnetic field the transition operator for electric-dipole radiation in the vector potential form is

$$H_I=(e/mc)\vec{A}\cdot\vec{p}+(e^2/2mc^2)\vec{A}\cdot(\vec{\mathcal{H}}\times\vec{r})+(e^2/2mc^2)A^2. \quad (39)$$

For later convenience we relate the matrix element of the above operator between an arbitrary S and P state to a corresponding matrix element obtained with the operator $\vec{A}\cdot\vec{r}$, $\vec{A}$ being the vector potential:

$$\langle nS|[(e/mc)\vec{A}_1\cdot\vec{p}+(e^2/2mc^2)\vec{A}_1\cdot(\vec{\mathcal{H}}\times\vec{r})]|n'P\rangle=(ie/\hbar c)[\epsilon_n-\epsilon_{n'}-\Delta]\langle nS|\vec{A}_1\cdot\vec{r}|n'P\rangle, \quad (40)$$

where ϵ_n and $\epsilon_{n'}$ are the energies in the absence of the magnetic field and $\Delta=e\hbar\mathcal{H}/2mc$. Here we have taken the vector potential associated with the external microwave field to be of the following form:

$$\vec{A}_1=a_1(\vec{\epsilon}_x-i\vec{\epsilon}_y)2^{-1/2}.$$

The decay amplitude for the ^2S level is now given by

$$T=\frac{\langle 2S|O_1|2P\rangle\langle 2P|O_2|1S\rangle}{\kappa-\hbar\omega_1-\Delta+\frac{1}{2}i\Gamma}+\sum_{n\neq 2}\frac{\langle 2S|O_1|nP\rangle\langle nP|O_2|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+\sum_{n=2}^{\infty}\frac{\langle 2S|O_2|nP\rangle\langle nP|O_1|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}, \tag{41}$$

where

$$O_1=(e/mc)\vec{A}_1\cdot\vec{p}+(e^2/2mc^2)\vec{A}_1\cdot(\vec{\mathcal{K}}\times\vec{r}) \tag{42}$$

and

$$O_2=(e/mc)\vec{A}_2\cdot\vec{p}+(e^2/2mc^2)\vec{A}_2\cdot(\vec{\mathcal{K}}\times\vec{r}). \tag{43}$$

Using the $e\vec{E}\cdot\vec{r}$ form of the interaction operator, we find that

$$T'=\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{\kappa-\hbar\omega_1-\Delta+\frac{1}{2}i\Gamma}+\sum_{n\neq 2}^{\infty}\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+\sum_{n=2}^{\infty}\frac{e^2\langle 2S|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}. \tag{44}$$

Writing $T=R+B$ and $T'=R'+B'$, the discrepancy between (41) and (44) is most pronounced when B and B' are dropped. Thus, squaring the resonant terms only, the transition probability resulting from R is proportional to

$$W\propto(\hbar\omega_1/\kappa+x)^2(x^2+\tfrac{1}{4}\lambda^2)^{-1}. \tag{45}$$

The one obtained from R' is proportional to

$$W'\propto(x^2+\tfrac{1}{4}\lambda^2)^{-1}, \tag{46}$$

where the dimensionless quantities x and y are found to be

$$x=(\kappa-\hbar\omega_1-\Delta)/\kappa \tag{47}$$

and

$$\lambda=\Gamma/\kappa. \tag{48}$$

The discrepancy is serious enough to alter the accepted value of the Lamb shift by one part in a thousand. Fortunately, (45) yields an asymmetrical line shape, while the shape given by (46) is symmetrical. Since the experimental curve favored the symmetrical form, Lamb chose the $e\vec{E}\cdot\vec{r}$ form of the interaction operator.[3] The issue can, however, also be decided on a theoretical basis, if we apply our previously gained understanding that the breakdown of the gauge transformation is due in part to the omission of the background terms. I proceed to show this. The starting point is the following identity (see Appendix):

$$\sum_{n=2}^{\infty}\frac{\langle 2S|O_1|n\rangle\langle n|O_2|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+\sum_{n=2}^{\infty}\frac{\langle 2S|O_2|n\rangle\langle n|O_1|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}=e^2\sum_{n=2}^{\infty}\frac{\langle 2S|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+e^2\sum_{n=2}^{\infty}\frac{\langle 2S|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}, \tag{49}$$

where O_1 and O_2 are defined in Eqs. (42) and (43) and the $2S$ and $1S$ are eigenstates of H_0 or H_0' without the Lamb term. Let S stand for the l.h.s. (or r.h.s.) of Eq. (49). We immediately recognize that to zeroth order in the Lamb operator there exists the following relationship between the background term B [the two sums in Eq. (41)] and S:

$$B-\left(\frac{e^2}{2mc^2}\right)\frac{\langle 2S|\vec{A}_1\cdot(\vec{\mathcal{K}}\times\vec{r})|2P\rangle\langle 2P|O_2|1S\rangle}{\Delta+\hbar\omega_1}=S. \tag{50}$$

Similarly, the background term B' [the sums in Eq. (44)] is related to S in the following manner:

$$B'-\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{\Delta+\hbar\omega_1}=S. \tag{51}$$

Combining Eqs. (50) and (51) we obtain

$$B=B'-\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{\Delta+\hbar\omega_1}+\left(\frac{e^2}{2mc^2}\right)\frac{\langle 2S|\vec{A}_1\cdot(\vec{\mathcal{K}}\times\vec{r})|2P\rangle\langle 2P|O_2|1S\rangle}{\Delta+\hbar\omega_1}. \tag{52}$$

It is shown in the Appendix that B' is of the order ω_1/ω_2, where ω_1 and ω_2 stand for the angular frequency of the microwave field and Lyman α, respectively. Hence for our purpose B' can be neglected; B, however, cannot be ignored. The next step is to replace the r.h.s. of Eq. (41) by $R+B$(approximate). Therefore,

$$T\approx\frac{\langle 2S|O_1|2P\rangle\langle 2P|O_2|1S\rangle}{\kappa-\hbar\omega_1-\Delta+\frac{1}{2}i\Gamma}-\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2P\rangle\langle 2P|\vec{E}_2\cdot\vec{r}|1S\rangle}{\Delta+\hbar\omega_1}+\left(\frac{e^2}{2mc^2}\right)\frac{\langle 2S|\vec{A}_1\cdot(\vec{\mathcal{K}}\times\vec{r})|2P\rangle\langle 2P|O_2|1S\rangle}{\Delta+\hbar\omega_1}. \tag{53}$$

Ignoring terms of order ω_1/ω_2, Eq. (53) assumes the simple form

$$T\approx-e^2\frac{(\epsilon_2+\Delta-\epsilon_0)}{(\hbar c)^2}\,\mathfrak{M}\left(\frac{\kappa-\Delta}{\kappa-\Delta-\hbar\omega_1+\frac{1}{2}i\Gamma}-1\right), \tag{54}$$

where $\mathfrak{M} = \langle 2S|\vec{A}_1 \cdot \vec{r}\,|2P\rangle\langle 2P|\vec{A}_2 \cdot \vec{r}|1S\rangle$. Introducing the dimensionless variables x and λ, the new transition probability is proportional to

$$W \propto [1 + (\Gamma/2\hbar\omega_1)^2]\,(x^2 + \tfrac{1}{4}\lambda^2)^{-1}. \tag{55}$$

The corrected transition probability yields a symmetric line shape whose maximum coincides with that of Eq. (46), which was obtained with the $e\vec{E}\cdot\vec{r}$ form of the electric-dipole interaction. The ratio of (55) to (46) is not quite unity: It deviates from 1 by one-tenth of a percent. Since absolute measurements are difficult to make, it is unlikely that one could put this to an empirical test. It is amusing that the agreement, at least concerning the position of the maximum, between the two forms for the transition probability is better in the case of a tunable weak external magnetic field than in the case of a frequency-tunable microwave field [cf. Eqs. (35) and (36)]. It behooves us now to comment upon the fact that, while for matrix elements without radiation damping exact agreement between the two forms of the perturbation expansion is obtained, provided only that stated conditions are fulfilled, in the case of linewidth formulas exact agreement is not obtained. One possible source of error may be the approximation made both in Sec. III and here when, computing the background terms, the unperturbed $2S$ wave function was used, i.e., the one degenerate with the $2P$ level. However, an order-of-magnitude estimate rules out this possibility; the error is more likely due to adding on the background terms to the Bethe-Lamb formula without including possible corrections in the resonant term induced by the background term.[10]

Roughly speaking, the problem is the following. In the derivation of the Bethe-Lamb or Weisskopf-Wigner formula it is assumed that the requirement of unitarity, i.e., that the sum of the probabilities adds up to one, is satisfied with the number of atomic levels included in the derivation (usually a finite number). Turning around and evoking the help of all (infinite) intermediate states to restore gauge invariance is therefore slightly inconsistent. Complete agreement is not to be expected. A systematic extension of the Weisskopf-Wigner level-width formula to include the (infinite) neighboring states and level shifts induced by radiative corrections can be carried through only with the aid of renormalization theory, as was shown some time ago by Low.[11] The electric-dipole interaction is of somewhat dubious value in such a program anyway.

It is now clear from the examples of Secs. III and IV that, while no detectable differences exist between the two forms of the dipole interaction when the background terms are properly included, the use of the $e\vec{E}\cdot\vec{r}$ form is at least computationally superior. Is this true generally? The answer is no. In Sec. V I supply a counterexample.

V. DOES $e\vec{E}\cdot\vec{r}$ YIELD BETTER APPROXIMATIONS?

In Secs. III and IV we saw that the use of $e\vec{E}\cdot\vec{r}$ led to computational simplicity. With a bit of hindsight, the reason for this is rather simple. Although the energy denominators in the background terms are always much larger than the energy denominator in the resonant part, with either form of the interaction operator, the numerators in the sums of Eqs. (20), (21), (41), and (44) are strongly gauge dependent. This can be easily surmised from the following typical example:

$$e\langle 2S|\vec{E}\cdot\vec{r}|nP\rangle = \pm(ie\omega/c)\langle 2S|\vec{A}\cdot\vec{r}|nP\rangle \tag{56}$$

and

$$(e/mc)\langle 2S|\vec{A}\cdot\vec{p}|nP\rangle = \frac{ie(\epsilon_2 - \epsilon_n)}{\hbar c}\langle 2S|\vec{A}\cdot\vec{r}|nP\rangle. \tag{57}$$

The ratio of (57) to (56) increases with increasing n, especially when the intermediate states are in the continuum. Hence, working with the electric field intensity one could by a simple comparison of the energy denominator in the resonant part with the smallest energy denominator in the background sum conclude that the neighboring levels could be ignored. Not so, however, with the vector potential, where the numerators in the background terms are much larger than the numerator in the resonant part of the amplitude. When the energy associated with the frequency of the radiation field is comparable with the energy separation of neighboring levels, the situation is not so clear cut. Consider, for instance, Rayleigh scattering off atomic hydrogen. The differential scattering cross section is

$$\frac{d\sigma}{d\Omega} = r_0^2\,|\mathfrak{M}|^2, \tag{58}$$

where r_0 is the classical electron radius,

$$\mathfrak{M} = \vec{\epsilon}\cdot\vec{\epsilon}' - \left(\frac{1}{m}\right)\left(\sum_n \frac{\langle 1S|\vec{\epsilon}\cdot\vec{p}|n\rangle\langle n|\vec{\epsilon}'\cdot\vec{p}|1S\rangle}{\epsilon_0 - \epsilon_n + \hbar\omega} + \sum_n \frac{\langle 1S|\vec{\epsilon}'\cdot\vec{p}|n\rangle\langle n|\vec{\epsilon}\cdot\vec{p}|1S\rangle}{\epsilon_0 - \epsilon_n - \hbar\omega}\right), \tag{59}$$

and $\vec{\epsilon}$ and $\vec{\epsilon}'$ are the (plane) polarization vectors of the incident and scattered photon, respectively. Working with the electric field intensity,

$$\mathfrak{M}' = -\omega^2 m\left(\sum_n \frac{\langle 1S|\vec{\epsilon}\cdot\vec{r}|n\rangle\langle n|\vec{\epsilon}'\cdot\vec{r}|1S\rangle}{\epsilon_0-\epsilon_n+\hbar\omega} + \sum_n \frac{\langle 1S|\vec{\epsilon}'\cdot\vec{r}|n\rangle\langle n|\vec{\epsilon}\cdot\vec{r}|1S\rangle}{\epsilon_0-\epsilon_n-\hbar\omega}\right). \quad (60)$$

$\mathfrak{M}$ and $\mathfrak{M}'$ are equal, as was shown by Dirac.[1] In the vicinity of a resonance the above expressions are not valid. We would expect them to be excellent approximations if $|\hbar\omega-(\epsilon_1-\epsilon_0)|\gg\Gamma$. Thus, for $|\hbar\omega-(\epsilon_1-\epsilon_0)|=10^{-2}\epsilon_0$, the amplitude should be accurate to within a correction no larger than 10^{-4}. In the spirit of the resonance approximation, we now replace $\mathfrak{M}$ with a one-level formula at

$$\hbar\omega=(0.75\pm 0.01)|\epsilon_0|.$$

To see which form of the transition operator will yield a more accurate value in the one-level approximation, we calculate both ways and compare the results with those obtained by Gavrila.[5] Writing $\mathfrak{M}$ as $\vec{\epsilon}\cdot\vec{\epsilon}'\,M(\hbar\omega)$, we obtain the following values for M:

$$M(0.74\epsilon_0)=-15.764, \quad M(0.76\epsilon_0)=15.383;$$
$$M_1(0.74\epsilon_0)=-15.608, \quad M_1(0.76\epsilon_0)=15.608;$$
$$M_2(0.74\epsilon_0)=-15.187, \quad M_2(0.76\epsilon_0)=16.026.$$

For this example at least, M_1, which was obtained with the vector potential, is a better approximation of M (Gavrila's result) than is M_2; M_2 was obtained by using the electric field intensity.

VI. CONCLUSION

To summarize, the following points were covered. To begin with, we found it necessary to draw a distinction between matrix elements without and with radiation damping. For the former, the necessary conditions for the equivalence of the two forms of the perturbation expansion were stated without proof. For the latter and, specifically, for the only known case (at least to this author) where the use of the vector potential leads to an apparent disagreement with experiment,[3] we were able to remove most of the discrepancy. The remaining disagreement between the forms of the Bethe-Lamb expression, though uninteresting from an experimental viewpoint, is nevertheless of theoretical interest. This was interpreted as an indication of the incompatibility between the standard Weisskopf-Wigner derivation of the level-width formula, in which the Hamiltonian of the material system is approximated by a finite number of levels, and the gauge transformation, which requires a complete set of states to restore equivalence.

In passing, I wish to make two additional comments. First, in any approximate calculation, one can use the requirement that the two forms of the perturbation expansion should be identical (at least for matrix elements without radiation damping) as a check on the accuracy of the approximation. If the two forms of the transition operator yield widely divergent results, the approximation may be a poor one. The second comment I wish to make is that in the Weisskopf-Wigner expression for the radiative decay of the $2P$ state of hydrogen where, again, one obtains a gauge-dependent expression for the level width, a large part of the discrepancy between the two forms of the line-shape formula[12] could be removed by including the excitation mechanism. After all, the validity of the standard assumption used in the derivation of the Weisskopf-Wigner formula—that at some initial time the atom is definitely in a $2P$ state—is somewhat questionable. Such an assumption may result in an inaccuracy of the order of the ratio of the level width to the energy of the Lyman α. And it is precisely of the same order of magnitude as the discrepancy between the use of the vector potential and the electric field intensity in the decay formula for the $2P$ state.[12] Since the problem here is of academic interest only, I refrain from working this out in detail.

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APPENDIX

Here it is shown that the transition amplitude for the decay of the $2S$ state of hydrogen via two photons in the presence of an external dc weak magnetic field is invariant under the gauge transformation, which eliminates the time-dependent vector potential and replaces it by the electric field intensity. The matrix element in terms of the vector potential is

$$T=\sum_{n=2}^{\infty}\frac{\langle 2S|O_1|n\rangle\langle n|O_2|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+\sum_{n=2}^{\infty}\frac{\langle 2S|O_2|n\rangle\langle n|O_1|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}, \tag{A1}$$

where in the presence of a magnetic field

$$O_i=(e/mc)\vec{A}_i\cdot\vec{p}+(e^2/2mc^2)\vec{A}_i\cdot(\vec{\mathcal{H}}\times\vec{r}), \tag{A2}$$

with the following polarizations for $\vec{A}_1$ and $\vec{A}_2$:

$$\vec{A}_1=a_1(\vec{\epsilon}_x-i\vec{\epsilon}_y)2^{-1/2},$$
$$\vec{A}_2=a_2(\vec{\epsilon}_x+i\vec{\epsilon}_y)2^{-1/2}.$$

Using the $e\vec{E}\cdot\vec{r}$ form of the transition operator,

$$T'=e^2\sum_{n=2}^{\infty}\frac{\langle 2S|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+e^2\sum_{n=2}^{\infty}\frac{\langle 2S|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}, \tag{A3}$$

where

$$\Delta=e\hbar\mathcal{H}/2mc. \tag{A4}$$

Simple calculations yield

$$\langle 2S|O_i|n\rangle=(ie/\hbar c)(\epsilon_2-\epsilon_n-\Delta)\times\langle 2S|\vec{A}_i\cdot\vec{r}|n\rangle \tag{A5}$$

and

$$\langle n|O_i|1S\rangle=(ie/\hbar c)(\epsilon_n+\Delta-\epsilon_0)\langle n|\vec{A}_i\cdot\vec{r}|1S\rangle. \tag{A6}$$

I will now proceed to show that $T=T'$, provided that

$$\epsilon_2-\epsilon_0=\hbar(\omega_1+\omega_2)$$

and that the summation is over a complete set of states. Substituting (A5) and (A6) into (A1), we get

$$T=\sum_{n=2}^{\infty}\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|n\rangle\langle n|\vec{E}_2\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_1}+e^2\sum_{n=2}^{\infty}\frac{\langle 2S|\vec{E}_2\cdot\vec{r}|n\rangle\langle n|\vec{E}_1\cdot\vec{r}|1S\rangle}{\epsilon_2-\epsilon_n-\Delta-\hbar\omega_2}$$
$$+(e^2\omega_1/\hbar c^2)\langle 2S|[(\vec{A}_1\cdot\vec{r}),(\vec{A}_2\cdot\vec{r})]|1S\rangle+(ie/\hbar c)\langle 2S|[(\vec{A}_1\cdot\vec{r}),O_2]|1S\rangle. \tag{A7}$$

Since the matrix element of the commutator of $[(\vec{A}_1\cdot\vec{r}),O_2]$ vanishes when the two states are orthogonal to each other, we have completed our proof. If we let Δ go to zero, we recover the result obtained by Zernik.[4] Let us proceed to compute T'. For $\omega_1/\omega_2\ll 1$, the procedure is rather simple. Performing the angular integrations in the r.h.s. of Eq. (A3), we obtain

$$T'=(1/3\epsilon_0)e^2a_0^2\vec{E}_1\cdot\vec{E}_2[\mathfrak{R}(\Omega_1)+\mathfrak{R}(\Omega_2)], \tag{A8}$$

where a_0 is the radius of the Bohr orbit and ϵ_0 is the ionization energy of hydrogen. The dimensionless expression $\mathfrak{R}$ is given by

$$\mathfrak{R}(\Omega)=\sum_{n=2}^{\infty}\int\int\frac{R_{20}(y)R_{n1}(y)y^3dy\,R_{n1}(y')R_{10}(y')(y')^3dy'}{\tilde{\epsilon}_2-\tilde{\epsilon}_n-\tilde{\Delta}-\Omega}, \tag{A9}$$

where $\tilde{\epsilon}_2$, $\tilde{\epsilon}_n$, $\tilde{\Delta}$, and Ω are the dimensionless quantities corresponding to ϵ_2, ϵ_n, Δ, and $\hbar\omega$, respectively, in units of $2\epsilon_0$. For our purpose, a simple way to compute $\mathfrak{R}(\Omega_1)$ and $\mathfrak{R}(\Omega_2)$ is the Laplace-transform method. Following Zernik,[13] we define

$$U_1(y,\Omega_1)=\sum_{n=2}^{\infty}y\frac{R_{n1}(y)\int R_{n1}(y')R_{20}(y')(y')^3dy'}{\tilde{\epsilon}_2-\tilde{\epsilon}_n-\tilde{\Delta}-\Omega_1} \tag{A10}$$

and

$$U_2(y,\Omega_2)=\sum_{n=2}^{\infty}\frac{yR_{n1}(y)\int R_{n1}(y')R_{10}(y')(y')^3dy'}{\tilde{\epsilon}_2-\tilde{\epsilon}_n-\tilde{\Delta}-\Omega_2}. \tag{A11}$$

$U_1(y,\Omega_1)$ satisfies the following differential equation:

$$y^2\left(\tilde{\epsilon}_2-\Omega_1-\tilde{\Delta}+\frac{1}{2}\frac{d^2}{dy^2}+\frac{1}{y}-\frac{1}{y^2}\right)U_1=R_{20}y^4, \tag{A12}$$

and similarly

$$y^2\left(\tilde{\epsilon}_2-\Omega_2-\tilde{\Delta}+\frac{1}{2}\frac{d^2}{dy^2}+\frac{1}{y}-\frac{1}{y^2}\right)U_2=R_{10}y^4. \tag{A13}$$

The derivation of these equations is based on the closure property of the P-state radial solutions of the homogeneous Schrödinger equation (see Ref. 13). Taking the Laplace transform of both equations, we get

$$(-\tfrac{1}{4}-2\tilde{\Delta}-2\Omega_1+p^2)\frac{d^2S_1}{dp^2}+2(2p-1)\frac{dS_1}{(dp)}=\frac{\sqrt{2}\;24(p-2)}{(p+0.5)^6} \tag{A14}$$

and

$$(-\tfrac{1}{4}-2\tilde{\Delta}-2\Omega_2+p^2)\frac{d^2S_2}{dp^2}+2(2p-1)\frac{dS_2}{dp}=96[p+1]^{-5}, \quad \text{(A15)}$$

where

$$S_1(p,\Omega_1)=\int_0^\infty U_1(y,\Omega_1)e^{-py}dy \quad \text{(A16)}$$

and

$$S_2(p,\Omega_2)=\int_0^\infty U_2(y,\Omega_2)e^{-py}dy. \quad \text{(A17)}$$

$\mathfrak{N}(\Omega_1)$ and $\mathfrak{N}(\Omega_2)$ can be obtained from the Laplace transforms by recognizing that

$$\mathfrak{N}(\Omega_1)=2\left(\frac{d^2S_1}{dp^2}\right)_{p=1} \quad \text{(A18)}$$

and

$$\mathfrak{N}(\Omega_2)=2^{-1/2}\left(\frac{d^2S_2}{dp^2}-\frac{1}{2}\frac{d^3S_2}{dp^3}\right)_{p=0.5}. \quad \text{(A19)}$$

Solving for S_1 and S_2 in a Taylor expansion around the points $p_0=(\frac{1}{4}+2\tilde{\Delta}+2\Omega_1)^{1/2}$ and $p_0'=(\frac{1}{4}+2\tilde{\Delta}+2\Omega_1)^{1/2}$, respectively, one obtains the following result

$$\mathfrak{N}(\Omega_1)\approx\frac{\sqrt{2}\,4!\,(\frac{2}{3})^4}{\tilde{\Delta}+\Omega_1}+\text{terms of order unity}$$

and $\mathfrak{N}(\Omega_2)$ is of order unity. Since B' [the two sums in Eq. (44)] is related to T' by

$$B'=T'+\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2p\rangle\langle 2p|\vec{E}_2\cdot\vec{r}|1S\rangle}{\Delta+\hbar\omega_1} \quad \text{(A20)}$$

and the leading term of T' is precisely

$$-\frac{e^2\langle 2S|\vec{E}_1\cdot\vec{r}|2p\rangle\langle 2p|\vec{E}_2\cdot\vec{r}|1S\rangle}{\Delta+\hbar\omega_1},$$

it follows that B' can be neglected. A similar result holds for the two sums in Eq. (21). The latter can be obtained by setting $\mathcal{K}=0$.

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