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A QUANTUM ELECTRODYNAMIC INVESTIGATION OF THE JAYNES-CRISP-STROUD APPROACH TO SPONTANEOUS EMISSION*

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ABSTRACT

Motivated by work of Jaynes and co-workers, the very old problem of atomic level shifts and level widths has begun to be re-examined recently. We have re-considered the question of level shifts and widths in spontaneous emission by a single two-level atom.

Our approach is not the customary one, although it is fully quantum electrodynamic. We show that if one follows the Jaynes-Crisp-Stroud line of argument and approximations, but integrates the relevant quantum electrodynamic equations instead of their semiclassical equations, one finds the following results: (1) Our predicted level width agrees with the semiclassical level width in the way that Jaynes has emphasized. (2) The level shift calculated by Jaynes and Crisp (called a Lamb shift by them) is reproduced exactly, when their same approximations are made. (3) There is, however, no frequency modulation of the emitted light. That is, the level shift is static, not a dynamic function of time.

It is interesting that the approach to semiclassical atomic radiation theory so long advocated by Jaynes, the direct self-consistent integration of dynamical equations over long times as opposed to perturbation analysis, is relatively easily taken over to quantum electrodynamics in this simple problem. We will comment on the results described above and contrast them with the results of a more careful quantum electrodynamic analysis.

(1) Introduction

Motivated by the work of Jaynes and co-workers,[1] the old problem of atomic level shifts and widths has recently begun to be re-examined. While QED is a highly successful theory (indeed the only workable field theory we have), it is still beset with self-energy infinities ultimately associated with the point-like nature of the electron. These are removed from the public view by the process of renormalization, in the hope that eventually some high frequency cut-off will be found to make the renormalization constants finite: such modifications proposed usually imply a radius to the electron. In the usual approach to QED, perturbation theory is used. Jaynes, prompted by the great progress made in theory and experiments on atoms interacting with electromagnetic fields, has re-investigated the problem of spontaneous emission by solving the relevant semiclassical equations of motion for the interacting field-atom system directly. An interesting product of such an approach (other than the novel time-dependence) is the non-appearance of divergences: the finite size of the atomic charge distribution removes the point-like singularity when retardation is taken into account.

We have adopted the approach advocated by Jaynes, but have applied it to the integration of the relevant quantum electrodynamic equations of motion instead of the Jaynes-Crisp-Stroud semiclassical equations. The field operators are then derived in terms of the source operators. We find the following results of this analysis: (1) our predicted level width agrees with the semiclassical width in the way Jaynes has emphasized; (2) the level shift calculated by Crisp and Jaynes (and called a Lamb shift by Stroud and Jaynes) is reproduced exactly when their same approximations are used; (3) the time evolution of the system agrees with the more usual methods of QED. In particular, there is no frequency chirping

of the emitted light, and the level shift is a static, not a dynamic function of time. Finally, the time evolution characteristics of semiclassical theory are obtained from the QED theory by decorrelating consistently the atom from the field operators when taking expectation values. It is interesting that the approach to semiclassical radiation theory, so long advocated by Jaynes, the direct integration of the equations of motion over long times, is relatively easily taken over to QED.

(2) The Equations of Motion

We take the Hamiltonian for a single bound two-level 'atom' interacting with a radiation field in pseudospin notation as

$$H = \frac{\hbar\omega_o}{2}\sigma_3 - \frac{\omega_o\mu}{c}\sigma_2 \int g(r)A_Z(r,t)d^3r \quad + \quad H_F \tag{1}$$

where g(r) represents the retardation effect[2] over the atomic charge distribution. In particular, for a hydrogenic atom transition from the $2P_Z$ to the 1S state (which represents the two levels, say, of our atom), g(r) is

$$g(r) = \frac{1}{(2\pi)^3}\int d^3k\, e^{i\vec{k}\cdot\vec{r}}\tilde{g}(k) = \frac{e^{-3r/2a}}{8\pi(2a/3)^3} \tag{2}$$

and $\tilde{g}(k) = (1 + \frac{4}{9}k^2a^2)^{-2}$.

The Heisenberg equations of motion for the atomic operators are

$$\dot{\sigma}_3 = \sigma_1 A(t) \tag{3}$$

$$\dot{\sigma}_2 = \omega_o\sigma_1 \tag{4}$$

$$\dot{\sigma}_1 = -\omega_o\sigma_2 - \sigma_3 A(t) \tag{5}$$

where we have defined $A(t) = (2\mu\omega_o/\hbar c)\int g(r)A_Z(r,t)d^3r$ for convenience. Defining the positive and negative frequency operators by

$$\sigma_1 \equiv \sigma^+ + \sigma^- \qquad \sigma_2 \equiv i(\sigma^- - \sigma^+) \tag{6}$$

$$A^{\pm}(r,t) \equiv \sum_\lambda \sqrt{\hbar}\ \frac{c}{2\pi} \int \frac{d^3k}{\sqrt{\omega_{k\lambda}}}\ \hat{\varepsilon}_{k\lambda}\ a_{k\lambda}^{\mp}(t)e^{\pm i\vec{k}\cdot\vec{r}} \tag{7}$$

(where $[a^-_{k\lambda}(t),\ a^+_{k'\lambda'}(t)] = \delta^3(k-k')\delta_{\lambda\lambda'}$, etc.), then (3) to (5) become, in the RWA (rotating wave approximation):

$$\dot{\sigma}_3 = \sigma^+ A^+ + A^-\sigma^- \tag{8}$$

$$\dot{\sigma}^+ = i\omega_o\sigma^+ - \tfrac{1}{2}A^-(t)\sigma_3 \tag{9}$$

$$\dot{\sigma}^- = -i\omega_o\sigma^- - \tfrac{1}{2}A^+(t)\sigma_3 \tag{10}$$

We derive the field, as do Jaynes and Crisp, from Maxwell's wave equation

$$\nabla^2 A^{\pm} - \frac{1}{c^2}\ddot{A}^{\pm} = -\frac{4\pi}{c}J_\perp^{\pm} \tag{11}$$

where the transverse current is defined by

$$J_\perp^{\pm} = \pm\frac{i\omega_o\mu}{(2\pi)^3}\sum_\lambda \sigma^{\mp}\int \hat{\varepsilon}_{k\lambda}\,\hat{\varepsilon}_{k\lambda}\cdot\hat{z}\,\tilde{g}(k)e^{i\vec{k}\cdot\vec{r}}d^3k \tag{12}$$

The formal solution

$$A_Z^{\pm}(r,t) = \pm\frac{i\ 4\pi c\mu\omega_o}{(2\pi)^3}\int_o^t dt'\sigma^{\mp}(t')\sum_\lambda\int d^3k\ \frac{e^{i\vec{k}\cdot\vec{r}}(\hat{\varepsilon}_{k\lambda}\cdot\hat{z})^2\tilde{g}(k)\sin\omega(t-t')}{\omega} \tag{13}$$

gives for the integral we need in the equations of motion the approximate result[3]

$$A^{\pm} \simeq A_o^{\pm} \pm 2i\Delta_c \sigma^{\mp}(t) - A\sigma^{\mp}(t) \tag{14}$$

where

$$A \equiv 4\omega_o^3\mu^2/3\hbar c^3 \quad \text{and} \quad \Delta_c \equiv \frac{5\omega_o^2\mu^2}{16\hbar a c^2}$$

where $A_o^{\pm}$ stand for the free-field homogeneous solutions.

(3) Solutions

We may now use (14) to write the atomic equations in terms of source operators entirely, except for the necessity of keeping the homogeneous solutions. The σ^- equation becomes:

$$\dot{\sigma}^- = -i\omega_o\sigma^- - \frac{\sigma_3}{2}\,[A_o^+ + (2i\Delta_c - A)\sigma^-],$$

using $\sigma_3\sigma^- = -\sigma^-$, valid for equal time operators, we obtain

$$\dot{\sigma}^- = [-i(\omega_o - \Delta_c) - \tfrac{A}{2}]\sigma^- - \frac{\sigma_3}{2}\,A_o^+ .$$

We take vacuum expectation values to eliminate the free fields, and get

$$\langle\dot{\sigma}^-\rangle_{vac} = \{-i(\omega_o - \Delta_c) - \tfrac{A}{2}\}\,\langle\sigma^-\rangle_{vac} \tag{15}$$

where the significance of both the Einstein A coefficient and the Crisp-Jaynes frequency shift is obvious. The solution of (15) is trivial:

$$\langle\sigma^-(t)\rangle_{vac} = \langle\sigma^-(o)\rangle_{vac}\, e^{-At/2}\, e^{-i(\omega_o - \Delta_c)t}, \tag{16}$$

and shows that Δ_c apparently plays the role of a transition frequency shift in QED as well as in the neoclassical theory. It is, however, not time-dependent in QED. The solution for $\langle\sigma_3(t)\rangle$ follows in the same way:

$$\langle\sigma_3(t)\rangle_{vac} = \{\langle\sigma_3(o)\rangle_{vac} + 1\}e^{-At} - 1 \tag{17}$$

showing the typical QED exponential decay of upper state occupation.

In semiclassical theory, on the other hand, the operator expectation values are used throughout and atom-field correlations are neglected: one takes

$$\langle\sigma^+ a_{k\lambda}\rangle_{vac} = \langle\sigma^+\rangle_{vac}\langle a_{k\lambda}\rangle_{vac}$$

and the equations of motion become, in the absence of external fields,

$$\langle\dot{\sigma}^-\rangle = -i\omega_o\langle\sigma^-\rangle - (i\Delta_c - \frac{A}{2})\langle\sigma_3\rangle\langle\sigma^-\rangle \tag{18}$$

$$\langle\dot{\sigma}_3\rangle = -2A\langle\sigma^+\rangle\langle\sigma^-\rangle \tag{19}$$

It is immediately obvious that the coefficients A and Δ_c are the same in both treatments. The semiclassical solutions[1] for $\langle\sigma_3\rangle$ and $\langle\sigma^-\rangle$ are

$$\langle\sigma_3(t)\rangle = -\tanh\frac{A}{2}(t-t_o) \tag{20}$$

$$\langle\sigma^-(t)\rangle = \frac{1}{2}\,\mathrm{sech}\,\frac{A}{2}(t-t_o)e^{-i(\omega_o t+\theta(t))} \tag{21}$$

where $\theta(t)$ represents the effects of a time-dependent frequency shift

$$\delta\omega(t) = \frac{d\theta}{dt} = -\Delta_c \tanh\frac{A}{2}(t-t_o) \tag{22}$$

Thus QED and semiclassical theory agree that the level width is A/2; and furthermore QED reproduces the Jaynes-Crisp shift Δ_c by making their same assumptions (RWA, etc.). Because of the correlated dynamics in QED there is no frequency chirping of the emitted light. The level shift is a static, not a dynamic function of time. At long times, of course, when the effects

of the atom-field correlations are no longer important, the theories agree in their time-evolution. However, these correlations play the role at short times of removing the metastable singular point of the semiclassical system. It is interesting that the shift Δ_c, common to both theories, does not agree with the usual Bethe formula, and more strikingly does not need renormalization or cut-offs. To see why this should be so, we analyze the relationship between Δ_c and the result of a more conventional QED calculation of level shifts.

(4) QED Frequency Shifts via Perturbation Theory

The usual QED treatment of level shifts uses the $\vec{p}\cdot\vec{A}$ interaction in second order perturbation theory and omits the A^2 terms as shifting all levels equally.[4] For our two-level atom, the QED shift of the upper (+) and lower (-) states would be

$$\hbar\Delta^{\pm} = P\sum_{\lambda}\int d^3k \frac{\langle 0_{k\lambda};\pm|\frac{e}{mc}\vec{p}\cdot\vec{A}|\mp;1_{k\lambda}\rangle\langle 1_{k\lambda};\mp|\frac{e}{mc}\vec{p}\cdot\vec{A}|\pm;0_{k\lambda}\rangle}{(E_{\pm} - E_{\mp} - \hbar ck)} \tag{23}$$

In the RWA $\Delta^- = 0$; and Δ^+ may be evaluated easily using a plane wave expansion of the field:

$$\hbar\Delta^{+} = +(\frac{e}{mc})^2(\frac{\hbar c}{4\pi^2})\, P\sum_{\lambda}\int \frac{d^3k}{k} \frac{\langle +|\vec{p}\cdot\hat{\varepsilon}_{k\lambda}\, e^{i\vec{k}\cdot\vec{r}}|-\rangle\langle -|\vec{p}\cdot\hat{\varepsilon}_{k\lambda}\, e^{-i\vec{k}\cdot\vec{r}}|+\rangle}{\hbar ck_o - \hbar ck} \tag{24}$$

where $\hbar ck_o = E_+ - E_-$.

In the conventional approach, the dipole approximation is used. Then (24) may be written (after doing the polarization sum and the angular integral)

$$\hbar\Delta^{+} = -\frac{2}{3\pi}\frac{\alpha}{m^2c^2}|\langle -|p|+\rangle|^2\int(1 - \frac{1}{1 - k/k_o})\hbar c\, dk \tag{25}$$

$$\equiv \delta m + \Delta_L$$

where we have followed common notation conventions. These terms are divergent: the linearly divergent δm term represents that part of the shift independent of binding and will be present for a free electron; it is concealed by renormalization of the electron's mass. The binding-dependent logarithmically divergent integral Δ_L is the Bethe part of the Lamb shift; it is usually cut-off on physical grounds[5] at mc/h.

It is not immediately obvious how these divergent usual results relate to the finite shift Δ_c. Let us follow the Jaynes-Crisp prescription and include retardation, then write Δ^+ in our previous notation as

$$\hbar\Delta^+ = -\frac{\omega_o^2\mu^2}{(2\pi)^2c^3}\cdot\frac{8\pi}{3}\ P\int_0^\infty (1-\frac{\omega_o}{\omega_o-\omega})(1+\frac{4}{9}\frac{\omega^2a^2}{c^2})^{-4}d\omega \qquad (26)$$

(The extra factor $(1+\frac{4}{9}\frac{\omega^2a^2}{c^2})^{-4}$ comes from the inclusion of retardation in the matrix elements, and we have converted matrix elements of $\vec{p}$ to those of the dipole moment $\vec{\mu}\equiv e\vec{r}$). So

$$\hbar\Delta^+ = -\frac{2}{3}\frac{\omega_o^2\mu^2}{\pi c^3}\cdot\frac{3c}{2a}\ P\int_0^\infty (1-\frac{x_o}{x_o-x})(1+x^2)^{-4}dx \qquad (27)$$

where $x_o = 2a\omega_o/3c$. Using the fact that $x_o \sim 10^{-3} \ll 1$, we find

$$\hbar\Delta^+ = -\frac{\omega_o^2\mu^2}{\pi c^2 a}\ [\frac{5\pi}{32}-\frac{11}{12}x_o + x_o\ln(\frac{1}{x_o}) + O(x_o^2)] \qquad (28)$$

Thus, due to the strong convergence supplied by retardation,[6] Δ^+ is now finite.

At this point two comments are required: (1) We know that the RWA has eliminated from consideration any integrals like (26), but with anti-resonant denominators $(\omega+\omega_o)^{-1}$. We have seen that the resonant integrals

have been cut off by retardation at $\omega \sim c/a \sim 10^3\omega_o$. Clearly if frequencies a thousand times greater than ω_o are important, we can't continue to ignore $2\omega_o$ contributions. The RWA is without justification in a level shift calculation and must be removed. We will do so promptly. (2) Note that the dominant term in the convergent Δ^+, the analog of δm in (25), is just

$$\Delta^+ => -\frac{5\omega_o^2\mu^2}{32ac^2\hbar} = -\frac{1}{2}\Delta_c, \tag{29}$$

exactly half the Jaynes-Crisp shift. In other words Δ_c seems to be most closely related to the part of the perturbative level shift which does not conventionally show up in the physical end result, due to renormalization. That this is so in our case too is easily verified by abandoning the RWA, calculating Δ^-, and finally taking the difference $\Delta^+ - \Delta^-$. The Δ_c parts cancel, and we are left with:

$$\delta\omega_{pert.} = \Delta^+ - \Delta^- = -\frac{A}{\pi}\left[\ell n\,\frac{3c}{2a\omega_o} - \frac{11}{12}\right] + O(x_o^2)\ . \tag{30}$$

The failure of our integration of the Heisenberg equations in Sec.(3) to give a frequency shift in agreement with (30) is interesting to consider. It is not due to a basic flaw in the method, but to our adoption of a conventional and superficial and incorrect identification of the positive and negative frequency parts of the field. The equation (14) should be replaced by

$$A^{\pm} \simeq A_o^{\pm} \pm 2i\Delta_c\sigma^{\mp}(t) - A\sigma^{\mp}(t) \mp i\{\Delta_c + \delta\omega_{pert.}\}\sigma_1 \tag{31}$$

where retardation has been retained, the RWA abandoned, and terms up to $O(x_o^2)$ kept in the evaluation of integrals. This expression, which one may obtain directly from the Hamiltonian given in (1) by use of the canonical commutation relations for the electromagnetic field, then leads to a solution like that in (16), but with Δ_c replaced by $\delta\omega_{pert}$. Both our approach, and the usual perturbative analysis, give the same quantum electrodynamic frequency shift.(7)

(5) Discussion and Conclusions

We have shown that Jaynes' program to obtain atomic level shifts and widths by integrating directly the semiclassical equations of motion, without resorting to perturbation theory, may be taken over to quantum electrodynamics fairly simply. A casual analysis of those QED equations (based on common assumptions, including the RWA) which correspond to the Jaynes-Crisp-Stroud equations, gives a frequency shift for the two-level transition identically equal to the Jaynes-Crisp shift. The shift is not time dependent, however.

A comparison with the usual perturbative QED result for the level shifts (whose difference is the frequency shift in question) then is seen to pose a number of questions. First of all, the perturbative shift is not equal to the Jaynes-Crisp shift. Second, one sees clearly that the effective cut-off provided by retardation is so high as to invalidate the RWA. Third, the closest correspondence to the Jaynes-Crisp shift formula is provided by the mass renormalization term in QED, just that term usually considered to have nothing to do with the transition frequency shift.

The conflict between the perturbative and non-perturbative QED results is resolved by giving up the Jaynes-Crisp approximations (RWA, etc.). A

correct identification of positive and negative frequency parts of the field operators shows that the shift obtained from the QED equation-of-motion approach agrees with the perturbative approach, and is essentially Bethe's result, albeit in the context of a fictitious two-level atom.

After all this is said, however, it must be recognized that Jaynes and co-workers are consciously constructing a new theory, not merely trying to do quantum electrodynamics differently. Thus the usual calculational procedures, and the usual interpretation of the various terms calculated, need have no relevance for them. Apart from comparison with experiment, the question of internal consistency of the theory becomes the only criterion for judgement. It seems to us that the use of the RWA is an important inconsistency. Apart from that objection, renormalization appears to raise the most urgent unanswered questions bearing on both the internal consistency of neoclassical theory, and on the magnitude of calculated level shifts.

It will be essential in any full appraisal of neoclassical theory to know at least whether neoclassical theory subscribes to Kramers' dictum that <u>all</u> theories are subject to renormalization of their "bare" component parts. It is well to keep in mind that the force of this dictum is <u>independent</u> of whether the "bare" quantities are finite or infinite. To be specific, for example, does the finite neoclassical level shift still contain a neoclassical free-electron part, presumably different from the δm part of (25), to be subtracted out in future refinements of the calculation? Perhaps it is still too early to expect detailed answers to questions of this kind.

References and Footnotes

1. M.D.Crisp and E. T. Jaynes, Phys. Rev. 179, 1253 (1969);
C. R. Stroud, Jr., and E. T. Jaynes, Phys. Rev. A1, 106 (1970).

2. We have directly verified by explicit calculation that all of the usual results of QED (including the divergent behaviour of the level shift) are obtained using the present method but neglecting retardation. However, retardation is the crucial factor in deriving the QED analogue of the Jaynes-Crisp level shift.

3. The integrals occurring in the evaluation of $A^{\pm}$ are of the same form as that in equation (26) and are performed using the same approximations. Such a derivation closely follows those of reference 1.

4. E. A. Power, 'Introductory Quantum Electrodynamics' (American Elsevier Pub. Co., 1965).

5. This is justified by the reduction in the degree of divergence found using a relativistic treatment, since at $\hbar ck \gtrsim mc^2$, pair states remove the high energy contribution to Δ_L which then becomes convergent; for the same reason δm becomes logarithmically divergent.

6. A result apparently well known in the older literature due to Waller shows that if one takes the non-relativistic formalism seriously and includes retardation and recoil energies, the free electron self-energy diverges only logarithmically. It is known that the corresponding Δ_L for a real hydrogen atom converges; Lamb has pointed out that this effectively cuts the integrals off at twice Bethe's cut-off and disagrees with experiment.
I. Waller, Zeits. für Phys. 62, 673 (1930).
N. M. Kroll and W. E. Lamb, Jr.,Phys. Rev. 75, 388 (1949).

7. It is amusing, but without physical significance, that if the RWA is imposed consistently on (31) then the (incorrect) result found by using the RWA in perturbation theory, $\delta\omega_{RWA} = \Delta^{+}$, is duplicated by our Heisenberg equation result.