Self-energy quantum electrodynamics: Multipole radiation

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Self-Energy Quantum Electrodynamics: Multipole Radiation[1]

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Within the context of Barut's self-field approach to quantum electrodynamics, we show that the exact relativistic expression for the Einstein A-coefficient of atomic spontaneous emission reduces, in the long wavelength approximation, to a form containing electric- and magnetic-like multipole contributions related to the transition charge and current distributions of the relativistic electron. A number of interesting features of the expressions involved are discussed, and their generalization to interacting composite systems is also pointed out.

1. INTRODUCTION

Within the framework of self-energy quantum electrodynamics (SEQED), advanced by Barut *et al.*,(1–6) spontaneous emission from one-electron atoms is treated as a self-energy attribute in a fashion close in spirit to the classical idea of radiation reaction. So far in this theory, only a first iteration of the action functional of the matter plus radiation field has been considered, in direct correspondence with first-order perturbation theory. Yet, to this order of iteration, account within the context of this approach has been made(4) of the electron's anomalous magnetic moment $(g-2)$, the Unruh and Casimir effects, the Lamb shift, and others, besides atomic spontaneous(5,6) emission and absorption.

The subject of this paper is also spontaneous emission. Encouraged by the success of our formulation in producing precise atomic decay rates for some of the low-lying hydrogenic excited states reported elsewhere,(5) we

[1] Dedicated to Prof. A. O. Barut, teacher and friend, on the occasion of his 65th birthday. I only hope it measures up to the man being honored.

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have recently employed[6] our general relativistic formula for the Einstein A-coefficient in a calculation of the decay rates of the $2S$ metastable hydrogenlike states of atoms and ions with values of the atomic number Z ranging between 1 and 92. Agreement between our results and those of other formulations as well as with experiment is good, especially for high Z values where a relativistic treatment is essential.

In this paper, we bring our exact formula[5] for the atomic transition rates one step closer to the familiar language and terminology of the standard theory. This goal is fulfilled by the retention, in the formula, of more terms than is usually done when the dipole approximation is adopted. We show that, in this regime, our expression, which was arrived at fully relativistically, reduces to a sum of terms formally similar to the ones one gets from contributions from all the electric and magnetic multipoles of the radiating system, namely the electron. We introduce a unified definition for the relativistic multipole moments in which the separation into electric and magnetic is made redundant. It will also be shown that contribution from the monopole term is automatically excluded. Finally, the same expression will be cast into a form reminiscent of the squared-amplitude language of the standard radiation theory.

2. THEORY

Within the context of SEQED, we have arrived at the following expression[5] for the Einstein A-coefficient of atomic spontaneous emission, or the transition probability per unit time for the decay of an atomic state n to a lower state s

$$\begin{aligned} A_{n\to s} &= -2\,\mathrm{Im}(\Delta E_{ns}) \\ &= -\frac{\pi}{2}\int \frac{d^3k}{k}\, T^{\mu}_{ns}(\mathbf{k})\, T_{sn}(-\mathbf{k})_{\mu}\, \delta(E_s - E_n + |\mathbf{k}|\partial) \\ &= -\frac{\pi\omega}{2}\int d\Omega_k\, T^{\mu}_{ns}(\mathbf{k})\, T_{sn}(-\mathbf{k})_{\mu}, \end{aligned} \tag{1}$$

where Im stands for *the imaginary part*, n and s stand for the totality of the respective states' quantum numbers n, l, J, and M, and natural units ($\hbar = c = 1$) are used. In the last step of Eq. (1) the radial integration over $|\mathbf{k}|$ has been carried out, resulting in the understanding that $|\mathbf{k}|$ is to be replaced everywhere by $\omega \equiv E_n - E_s$, by virtue of the delta function. Moreover, $d\Omega_k = \sin\theta_k\, d\theta_k\, d\phi_k$ and the quantities

$$T^{\mu}_{ns}(\mathbf{k}) = \int \frac{d^3r}{(2\pi)^{3/2}}\, J^{\mu}{}_{ns}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}} \tag{2}$$

are Fourier transforms, or transition form factors, of the electron current

$$J^{\mu}_{ns}(\mathbf{r}) = -e\bar{\psi}_n(\mathbf{r})\,\gamma^{\mu}\psi_s(\mathbf{r})$$
$$= -e(\rho_{ns}, \mathbf{J}_{ns}) \tag{3}$$

The wave functions ψ are, everywhere, the well-known exact solutions of the Dirac equation for a single electron in the Coulomb field of the atomic nucleus and $\bar{\psi}$ is the Dirac adjoint of ψ.

Equation (1) is thus exact and has been the basis of our decay rate calculations referred to above. At this point, however, we would like to distinguish between two levels of approximation. First, the dipole limit, on the basis of which most decay rates to date have been reported, is achieved by replacing the exponential factor in Eq. (2) by unity. Equation (1) has been shown[(5)] to reduce, in this limit, to its well-known nonrelativistic counterpart. Although retaining only the dipole term is believed to the sufficient for most purposes in atomic physics calculations, this may turn out to be too severe for radiation from atoms with high values of the atomic number Z, where the relativistic corrections become important. It may also prove to be equally as severe for calculations involving the properties of atomic Rydberg states, where the atomic dimensions are typically of the order n^2a_0, with n the principal quantum number (which can be quite large) and a_0 the Bohr radius.

At a second level, when the *long wavelength approximation*,[2] to be described shortly, is adopted,[(7,8)] a familiar picture begins to emerge. We shall demonstrate that the decay rate formula reduces to a sum of contributions from objects formally related to the classical electric and magnetic multipoles of the system, to all orders. In this way, some degree of resemblance will be established between Barut's fully relativistic semiclassical formulation and the familiar theory of nonrelativistic multipole radiation from atoms.

The starting point for the reduction of Eq. (1) to meet the conditions of the above-mentioned approximation is the observation that $T^{\mu}_{sn}(-\mathbf{k}) = T^{\mu}_{ns}(\mathbf{k})^{\dagger}$. Equation (1) can then be written in expanded form as

$$A_{n\to s} = -\frac{\pi\omega}{2}\int d\Omega_k\{|T^0_{ns}(\mathbf{k})|^2 - |\mathbf{T}_{ns}(\mathbf{k})|^2\} \tag{4}$$

[2] Emphasis is added to point to the well-known fact that the basis for both approximations is one and the same, namely, that the radiation wavelength be large compared with the atomic dimensions.

Next we look at

$$T^0_{ns}(\mathbf{k}) = -e\int \frac{d^3r}{(2\pi)^{3/2}}\,\bar{\psi}_n(\mathbf{r})\,\psi_s(\mathbf{r})\,e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= -\frac{4\pi e}{(2\pi)^{3/2}}\sum_{lm} i^l Y^*_{lm}(\hat{k})\int d^3r\, g_l(\omega r)\, Y_{lm}(\hat{r})\,\rho_{ns}(\mathbf{r}) \tag{5}$$

where use has been made of the following expansion for the exponential term in terms of spherical Bessel functions $g_l(\omega r)$ and spherical harmonics Y_{lm}

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l g_l(\omega r)\, Y_{lm}(\hat{r})\, Y^*_{lm}(\hat{k}) \tag{6}$$

and where

$$\rho_{ns}(\mathbf{r}) = \bar{\psi}_n(\mathbf{r})\,\psi_s(\mathbf{r}) \tag{7}$$

As is well known from the standard textbooks[7,8] of quantum mechanics, the *long wavelength approximation* amounts to retaining only the first term in the power series expansion of the spherical Bessel function

$$g_l(\omega r) \approx \frac{(\omega r)^l}{(2l+1)!!} \tag{8}$$

When (8) is put back into (5), we obtain

$$T^0_{ns}(\mathbf{k}) \approx \frac{e}{\sqrt{2\pi^2}}\sum_{lm}(-1)^{m+1}\frac{\sqrt{2l+1}}{(2l+1)!!}(i\omega)^l Y^*_{lm}(\hat{k})(Q_{l,-m})_{ns} \tag{9}$$

where

$$(Q_{lm})_{ns} \equiv \sqrt{\frac{4\pi}{2l+1}}\int \rho_{ns}(\mathbf{r})\, r^l Y^*_{lm}(\hat{r})\, d^3r \tag{10}$$

are transition matrix elements of the quantities

$$Q_{lm} \equiv \sqrt{\frac{4\pi}{2l+1}}\, r^l Y^*_{lm}(\hat{r}) \tag{11}$$

Proceeding basically along the same lines, as has been done to arrive at Eq. (9) for the scalar objects, the vector quantities in the main decay rate formula can be put into the following form:

$$\begin{aligned}\mathbf{T}_{ns}(\mathbf{k}) &= \int \frac{d^3r}{(2\pi)^{3/2}} \mathbf{J}_{ns}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= -\frac{4\pi e}{(2\pi)^{3/2}} \sum_{lm} i^l Y^*_{lm}(\hat{k}) \int d^3r\, g_l(\omega r)\, Y_{lm}(\hat{r})\, \mathbf{J}_{ns}(\mathbf{r}) \\ &\approx \frac{e}{\sqrt{2\pi^2}} \sum_{lm} (-1)^{m+1} \frac{\sqrt{2l+1}}{(2l+1)!!} (i\omega)^l\, Y^*_{lm}(\hat{k})(\mathbf{Q}_{l,-m})_{ns} \end{aligned} \tag{12}$$

In Eq. (12),

$$(\mathbf{Q}_{lm})_{ns} \equiv \sqrt{\frac{4\pi}{2l+1}} \int \mathbf{J}_{ns}(\mathbf{r})\, r^l Y^*_{lm}(\hat{r})\, d^3r \tag{13}$$

are transition matrix elements of the quantities

$$\mathbf{Q}_{lm} I \equiv Q_{lm} \boldsymbol{\gamma} \tag{14}$$

$\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \gamma_3)$ are the familiar Dirac gamma matrices, and I is the 4×4 identity matrix. Furthermore, we have taken the transition probability current as

$$\mathbf{J}_{ns}(\mathbf{r}) = \bar{\psi}_n(\mathbf{r})\, \boldsymbol{\gamma} \psi_s(\mathbf{r}) \tag{15}$$

Note at this stage that the classical objects defined by Eqs. (11) and (14) form the components of a four-vector

$$Q^{\mu}_{lm} = (Q_{lm}, \mathbf{Q}_{lm}) \tag{16}$$

We call $-e(Q^{\mu}_{lm})_{ns}$ the *relativistic* (quantum mechanical) *multipole moments* of the electron. This is justified as follows. In the program of SEQED, Schrödinger's interpretation of the wave function is adopted, whereby $\rho = -e|\psi|^2$ is the real charge density of the electron. Within the context of this interpretation, $\rho_{ns}(\mathbf{r})$ is the charge associated with the electron transition $n \to s$ in the (external) Coulomb field of the atomic nucleus. Recall that the textbook[7–9] definition of the multipole moments of a classical charge distribution of density ρ is

$$q_{lm} = \sqrt{\frac{4\pi}{2l+1}} \int \rho(\mathbf{r})\, r^l Y^*_{lm}(\hat{r})\, d^3r \tag{17}$$

apart from the multiplicative factor upfront in some places. With all of this in mind and provided we take $-e\rho_{ns}(\mathbf{r})$ as a transition density for the electronic charge distribution, our (quantum mechanical) interpretation of the quantities $-e(Q^{\mu}_{lm})_{ns}$ becomes all too obvious.

Now we insert (9) and (12) back into (4) and carry out the remaining trivial integration over the **k**-space angles, arriving finally at

$$\begin{aligned} A_{n\to s} &\approx -\frac{e^2}{4\pi}\sum_{lm}\frac{2l+1}{[(2l+1)!!]^2}\,\omega^{2l+1}\{|(Q_{l,-m})_{ns}|^2-|(\mathbf{Q}_{l,-m})_{ns}|^2\} \\ &= -\frac{e^2}{4\pi}\sum_{lm}\frac{2l+1}{[(2l+1)!!]^2}\,\omega^{2l+1}(Q^{\mu}_{l,-m})_{ns}(Q_{l,-m\mu})_{ns} \end{aligned} \tag{18}$$

Within the same context, and using the same language as before, we call the expression given in Eq. (18) *the probability of* 2^{l+1}*-pole radiation.* The basis for this choice of nomenclature will be further highlighted in the discussion below. In the meantime, readers not at ease with this slight abuse of language are invited to make the (legitimate) transformation $l \to l-1$ in the series (18) and to keep using the same standard terminology, whereby $l=1$ gives the dipole term, $l=2$ the quadrupole term, and so on. While the suggested change of dummy index will keep the predictive power of the formula intact, it will still automatically exclude contribution from the $l=0$ term. This exclusion evolves naturally from the mathematics, in addition to being justified on sound physical grounds. More on this will be given in the discussion section.

Before moving on to the next section, we would like to remark that Eq. (18) can be easily generalized to the case of N interacting particles. All that needs to be done[7] is express the transition charge and current densities in terms of the wave functions of the composite system in question.

3. DISCUSSION AND CONCLUSIONS

Let us begin the discussion by taking up the question of whether the dipole formula can be recovered from the series (18) of the previous section. The first term in the sum corresponds to $l=0$. We have no choice but to take it as such. We now show that the $l=0$ term is indeed the probability of (electric) dipole radiation, in light of the fact that departure from the dipole limit has been efected by Eq. (8) for the spherical Bessel functions. Note that setting $l=0$ in (8) and working backwards to (6) leads naturally to the desired limit.

The proof is carried out in two steps. First, the (relativistic) Dirac wave functions are to be replaced with their (nonrelativistic) Schrödinger counterparts. An immediate consequence of this is to lose the electron spin. We make up for this by multiplying the result by a factor of 2, as has been explained elsewhere.[5,10] Second, the photon polarization will be brought into the picture according to the prescription of the standard theory. The result of all this will be the dipole term in full glory, complete with the famous factor 4/3, the selection rules and all.

With $l=0$, Eq. (18) yields

$$A_{n\to s}(\text{dipole}) = -\frac{e^2}{4\pi}\,\omega\{|(Q_{00})_{ns}|^2 - |(\mathbf{Q}_{00})_{ns}|^2\} \tag{19}$$

From (10) and orthogonality of the wave functions, we get

$$(Q_{00})_{ns} \to \int \psi_n^\dagger \psi_s \, d^3r = 0 \tag{20}$$

Furthermore, Eqs. (11), (13), and (14) lead to

$$(\mathbf{Q}_{00})_{ns} = \int \psi_n^\dagger \boldsymbol{\alpha} \psi_s \, d^3r \to \mathbf{v}_{ns} \tag{21}$$

where $\mathbf{v}_{ns}$ is the transition matrix element of the velocity operator which can be expressed, in the Heisenberg picture, in terms of the matrix element of the position vector of the electron as

$$\mathbf{v}_{ns} = -i\omega \mathbf{r}_{ns} \tag{22}$$

With (20)–(22) inserted back into (19), we have

$$\begin{aligned} A_{n\to s}(\text{dipole}) &= \frac{e^2}{4\pi}\,\omega^3 |\mathbf{r}_{ns}|^2 \\ &= \frac{1}{4\pi}\,\omega^3 |\mathbf{d}_{ns}|^2 \end{aligned} \tag{23}$$

where the dipole moment operator is $\mathbf{d} \equiv -e\mathbf{r}$. At this point, we follow the textbooks in introducing the photon polarization, summing over polarization states and integrating over all spatial directions. Remembering to multiply by a factor of 2 to account for the lost electron spin, the result of all this, in natural units, will be

$$\begin{aligned} A_{n\to s}(\text{dipole}) &= 2\frac{1}{4\pi}\,\omega^3 \sum_{\lambda=1}^{2} \int |\mathbf{e}_\lambda \cdot \mathbf{d}_{ns}|^2 \, d\Omega \\ &= \frac{4}{3}\,\omega^3 |\mathbf{d}_{ns}|^2 \end{aligned} \tag{24}$$

The second point in this section concerns the monopole term. We find the absence of this term from our theory particularly interesting and consistency of this rigorous prediction with classical radiation theory quite remarkable. For the sake of comparison and contrast, we quote,[7] below, the probability of electric multipole radiation (in the same system of units as we have, so far, been using)

$$W_{n\to s}=\frac{e^2}{4\pi}\sum_{lm}\frac{2(2l+1)(l+1)}{l[(2l+1)!!]^2}\,\omega^{2l+1}\,|(Q_{l,-m})_{ns}|^2 \tag{25}$$

Equation (25) is derived within the context of conventional QED using the same approximation as has been introduced by Eq. (8) above. For $l=1$, this formula reduces to the probability of electric dipole radiation. Whereas, if one naively sets $l=0$ in it, one gets

$$W_{n\to s}=\frac{0}{0} \tag{26}$$

an indeterminate quantity. Yet, standard QED does not tell us anything about this potential drawback, apart possibly from the remark that $J_n=0\to J_s=0$ transitions are absolutely ruled out by the transverse nature of the radiation field. This may be added to the list of mathematical inconsistencies that beset the foundations of conventional QED. As a side to this problem, we would like to add that, in arriving at (25), an *arbitrary* normalization constant for the photon wavefunction is used,[7] chosen as $-\sqrt{(l+1)/l}$ to make things right for the case of $l=1$.

In conclusion:

- We have expressed the Einstein A-coefficient of spontaneous emission, within the context of SEQED, in terms of suitably defined relativistic radiating multipoles.
- We have rigorously shown that the monopole term is entirely out of the picture.
- The dipole approximation has been fully recovered and corresponds to the first term in the series ($l=0$).

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