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Gauge invariance and photon emission from ground state atoms in the presence of external electromagnetic field

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Abstract.—The relevance of gauge invariance in considering the question of emission of photons in the presence of external electromagnetic field from the ground state of quantum mechanical systems is studied. With an exact numerical calculation for atomic hydrogen, it is shown that the photons cannot be unequivocally assigned to have been emitted from the ground state due to the invariance of gauge of the probability for the process.

There are various processes involving external electromagnetic waves in which the lowest order term in the perturbation is given by two different amplitudes which have to be calculated separately. One of the more typical example is the Raman-like processes which are described by the two diagrams in figure 1.

The first of these two diagrams corresponds to absorption of a photon $\omega_L$ by the atom in the initial state $|i\rangle$ followed by spontaneous emission of a photon $\omega_S$, the atom being found in the final state $|f\rangle$. The other diagram corresponds to taking the absorption and the emission process being reversed in order.

Another usual picture of the process is provided by the energy-level diagrams in figure 2 where figure 2a and figure 2b correspond respectively to figure 1a and figure 1b.

In the course of a recent investigation on such processes we were led to ask the following question: can one place oneself under the condition in which one of the two amplitudes associated with these diagrams becomes vanishingly small? More precisely, if the contribution of the diagram in figure 1a (or Fig.2a) vanishes, could one observe the rather unusual one-photon spontaneous emission from the ground state? Obviously, such an emission process of a photon $\omega_S$ can only take place in the presence of an external field with photons belonging to a mode with frequency $\omega_L = E_f - E_i + \omega_S$ (atomic units will be used throughout this letter). The answer to this question requires accurate evaluation of second-order perturbative am-
plitudes. For most systems this entails approximations with the notable exception of hydrogen atom where the Coulomb Green’s function being known, an exact non-relativistic calculation can be done [1-4]. We shall treat specifically the Raman process between 1S and 2S states of hydrogen.

The amplitudes of interest here are:

\[
\begin{align*}
T^I_{1S-2S} &= (2S| H^+_{\text{int}}(\omega_3) G(E_{1S} + \omega_L) H_{\text{int}}(\omega_L) |1S) \\
T^{II}_{1S-2S} &= (2S| H^+_{\text{int}}(\omega_L) G(E_{1S} + \omega_S) H_{\text{int}}(\omega_S) |1S)
\end{align*}
\]

(1)

(2)

Fig.2.- Energy level diagrams associated with (Stokes-) Raman scattering. Figure 2a (2b) corresponds to the Feynman diagrams figure 1a (1b) respectively.

Where \(G\) is the Coulomb Green’s function and \(H_{\text{int}}(\omega_L)\) represents the interaction Hamiltonian associated to the absorption of the incoming photon with frequency \(\omega_L\) and \(H^+_{\text{int}}(\omega_S)\) corresponds to the emission of the scattering photon with frequency \(\omega_S\). We have performed two independent calculations of these amplitudes, using two different forms of the interaction Hamiltonian written either in the p- or r-gauge. Within the framework of the non-relativistic, dipole approximation our computation is exact, i.e. we have computed exactly the amplitudes given in equation (1) and (2) by using compact representations of the Coulomb Green’s function [1-4].

The differential cross section, in the r-gauge, is given by:

\[
\frac{d\sigma}{d\Omega} = \gamma^2_0 \omega_L \omega_S^3 (\vec{e}_S \cdot \vec{e}_L)^2 |M^I + M^{II}|^2
\]

(3)

where \(r_0\) is the classical radius of the electron, \(\vec{e}_L\) and \(\vec{e}_S\) are the polarization vectors of the photons and \(M^I\) and \(M^{II}\) are the following dimensionless second-order atomic amplitudes:

\[
\begin{align*}
M^I &= (2S| rG(E_{1S} + \omega_L) |1S) \\
M^{II} &= (2S| rG(E_{1S} - \omega_S) |1S)
\end{align*}
\]

(4a)

(4b)

If one uses instead the p-gauge one has:

\[
\frac{d\sigma}{d\Omega} = \gamma^2_0 \omega_L \omega_S^3 (\vec{e}_S \cdot \vec{e}_L)^2 |M^P + M^{II}|^2
\]

(5)

where \(M^I\) and \(M^{II}\) have the same form than \(M^P\) and \(M^{II}\) except that \(r\) is substituted by \(p\). The calculation of the differential cross-section has been done in the frequency range 0.4 a.u. \((\omega_L = 0.48 \text{ a.u.)}\) (with the particular geometry \(\epsilon_L / \epsilon_S\)) since this is the frequency range pertinent to our problem. Our results agree with previous calculations conducted along the same lines [5,6]. (We do not display these cross-sections since they are already in the literature).

One first observes that the cross-section is gauge independent as it must be [7,8]. One notes also, as several authors did in similar instances, [5,6] that the cross-section vanishes for an infinite set of frequencies located between two consecutive resonances. For instance, the first two zeroes of the cross section are located at \(\omega_L = 0.45636 \text{ a.u. and } \omega_L = 0.47439 \text{ a.u.}\). Such zeroes appear due to the fact that the amplitude (written in either gauge) \(M^I\) goes through zero near, but not exactly at, these frequencies. For instance \(M^P_1\) is zero (i.e. changes of sign) at \(\omega_L = 0.45576 \text{ a.u.}\) and at this frequency:

\[
(M^I_1 + M^{II}_1) |_{\omega_L = \omega_L^0} = M^{II}_1 |_{\omega_L = \omega_L^0}
\]

(6)

One, however, notes the following interesting fact: the corresponding amplitude \(M^P_1\), written in the p-gauge, does not vanish at the same frequency (see Fig.4). Indeed, it is zero at \(\omega_L^1 = 0.45738 \text{ a.u.} \neq \omega_L^0\) and at this frequency one has:

\[
(M^I_1 + M^{II}_1) |_{\omega_L = \omega_L^1} = M^{II}_1 |_{\omega_L = \omega_L^1}
\]

(7)

Thus, the frequency at which \(M^I\) goes through zero is gauge-dependent. This is a direct consequence of the fact that the gauge equivalence is valid for the sum \(M^I + M^{II}\) and not for a single amplitude \(M^I\) or \(M^{II}\). More precisely one should have [7]:

\[
M^I + M^{II} = (\omega_L \omega_S) (M^P + M^{II})
\]

(8)

Now, when the contributions of the diagram figure 1a is zero, referring to figure 2a, we may say that all the photons \(\omega_S\) detected come from the spontaneous emission of the ground state. However, one cannot locate a critical frequency \(\omega_S^0\) at which the photons emitted come entirely from the ground state. That statement can be made for \(\omega_S^0 = 0.08236 \text{ a.u.}\) but only in r-gauge or for \(\omega_S^0 = 0.08088 \text{ a.u.}\) but only in p-gauge ! [9].

We are led to an apparently paradoxical result. This paradox cannot be resolved without additional hypothesis. If one could adduce further arguments for choosing a particular gauge, one would be able
Fig. 3.- Variations of the dimensionless atomic matrix elements $M_\ell^I$ (full line) and $M_\ell^H$ (broken line) in terms of the external frequency $\omega_L$. Note that, for convenience, the signs of the amplitudes have been changed and an angular factor of $1/3$ has been inserted. The arrows indicate the positions of the $(1s-3p)$ and $(1s-4p)$ resonance.

Fig. 4.- Variations of the dimensionless amplitude $M$ written in either gauges, in the vicinity of the first zero of the cross section at $\omega_L = \omega_0 = 0.45536$ a.u. For the sake of comparison we have reported the matrix elements $M_\ell^I, M_\ell^H, (\omega_L\omega_0)^{-1} M_\ell^I$ and $(\omega_L\omega_0)^{-1} M_\ell^H$ and the overall amplitude $M = M_\ell^I + M_\ell^H$ which is invariant i.e. $M_\ell^I + M_\ell^H = (\omega_L\omega_0)^{-1} (M_\ell^I + M_\ell^H)$. Again, for convenience, the signs of the amplitudes have been changed. (---) : $M_\ell^I$; (-----) : $M_\ell^H$; (-----) : $M_\ell^I$; (-----) : $(M_\ell^I + M_\ell^H)$.

to state that all the emitted photons originate from the ground state at a particular frequency. In the absence of any fundamental reason for a preferential gauge, one has to give up the possibility of being able to choose a physical condition, i.e. a frequency for our case, in which one of the two amplitudes vanishes.

We are led from this study of the hydrogenic 1S-2S Raman effect to the following conclusions. There exists frequencies, located close to the zeroes of the cross section, at which the emission from the ground state is the only source of the Raman photons. However, this statement is gauge dependent. There is an "gauge anomaly" regarding the privileged frequency of spontaneous emission from the ground state in the presence of an external field. Our conclusions can be extended to an infinite set of frequencies lying between resonances in hydrogen. Note also that analogous statements may be made for the symmetrical process involving the spontaneous emission for the metastable 2S state, the role of the frequencies $\omega_S$ and $\omega_L$ being interchanged (anti-Stokes Raman scattering). Note finally that similar analysis can be performed when considering other photon scattering processes such as Rayleigh scattering. We also estimate that the paradox would survive even with a more refined analysis taking into account for instance retardation or relativistic corrections.

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