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LETTER TO THE EDITOR

# A quantum calculation of the higher order terms in the Bloch–Siegert shift

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**Abstract.** We present a fully quantum mechanical calculation of the higher order terms in the Bloch–Siegert shift. Contrary to Cheng and Stehle's QED calculation, our results are in complete agreement with those of semi-classical approaches, as can be expected in the RF domain.

Several papers have recently been devoted to the calculation of higher order terms appearing in the expression of the Bloch–Siegert shift. This renewal of interest has been stimulated by an article of Chang and Stehle (1971) who derive the shift from a quantum electrodynamics calculation.

The expression obtained by Chang and Stehle is in complete disagreement with the results of several other theoretical approaches: Shirley's theory (1965), using Floquet states, Pegg and Series' treatment (1970, 1973, see also Pegg 1973), based on appropriate changes of reference frames, Stenholm's calculations (1972), leading to continued fractions.

One could think that the origin of the discrepancy lies in the difference of treatment of the RF field, which is described quantum mechanically in Chang and Stehle's theory, classically in the others. We present in this note a simple calculation of the higher order terms in the Bloch-Siegert shift, using a quantum description of the RF field ('dressed' atom theory: see Cohen-Tannoudji 1968, Haroche 1971), and giving results in complete agreement with those of the semiclassical approaches. This is not surprising: in the RF domain, the average number of photons is very large, so that the pure quantum effects are negligible.

To calculate the Bloch–Siegert shift up to sixth order we use the formalism and the notations of Haroche (1971). The eigenstates of the unperturbed hamiltonian:

$$H_0 = \omega_0 J_z + \omega a^+ a \tag{1}$$

are the states $|\pm, n\rangle$, of energy $\pm\omega_0/2 + n\omega$, represented by the dotted lines of figure 1 ($|\pm\rangle$ are the states of the spin in $\boldsymbol{J}$ the static field $\boldsymbol{B}_0$ parallel to O$z$, $\omega_0$ is the Larmor frequency in $\boldsymbol{B}_0$, $n$ is the number of RF quanta of frequency $\omega$, $a^+$ and $a$ are the creation and annihilation operators of a RF photon). The RF field has a linear polarization, parallel to O$x$, and its coupling with the spin is described by:

$$H_1 = \frac{\lambda}{2}(J_+ + J_-)(a^+ + a). \tag{2}$$

$H_1$ perturbs the energy levels and leads to the diagram represented by the full lines of figure 1; $n$ is very large, and it may be shown that the coupling constant $\lambda$ of equation (2) is related to the Larmor frequency $\omega_1$ associated to the classical RF field amplitude by:

$$\lambda = \frac{\omega_1}{2\sqrt{n}}. \tag{3}$$

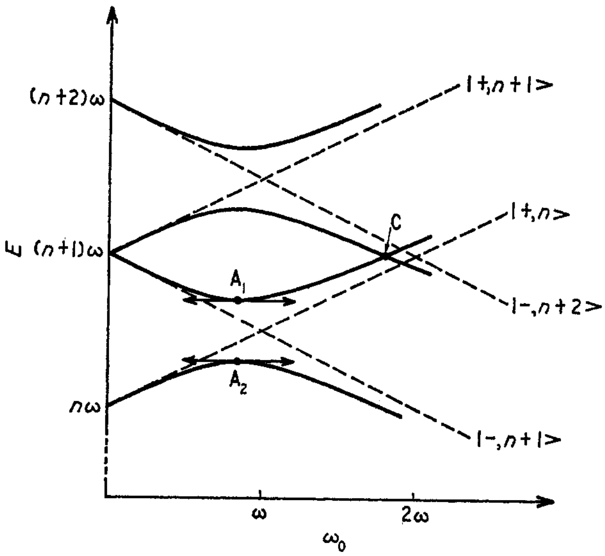


**Figure 1.** Energy levels of the system 'spin+RF photons'.

The various magnetic resonances observable on the spin correspond to the 'anti-crossings' and 'crossings' appearing on figure 1. Particularly, it may be shown that the centre of the resonance we are interested in, is given by the abscissa of the points $A_1$ and $A_2$ where the energy levels of figure 1 have a zero slope (centre of the first anti-crossing).

Let us call $|a\rangle = |+, n\rangle$ and $|b\rangle = |-, n+1\rangle$ the two unperturbed levels corresponding to this anticrossing. The perturbed energy levels are *exactly* given by the implicit equation:

$$[E-E_a-R_{aa}(E,\omega_0)][E-E_b-R_{bb}(E,\omega_0)]-|R_{ab}(E,\omega_0)|^2 = 0 \tag{4}$$

where $E_a = \frac{1}{2}\omega_0$, $E_b = \omega-\frac{1}{2}\omega_0$ (substracting the constant $n\omega$ to every energy),

$$R(E,\omega_0) = PH_1P + \sum_{n=1}^{\infty} PH_1\left(\frac{Q}{E-H_0}H_1\right)^n P$$

with $P = |a\rangle\langle a|+|b\rangle\langle b|$, $P+Q = 1$. $R_{ab}$ contains only one term, and does not depend on $E$ and $\omega_0$:

$$R_{ab} = \tfrac{1}{2}\lambda\sqrt{n} = \tfrac{1}{4}\omega_1. \tag{5}$$

Equation (4) then becomes:

$$[E-\tfrac{1}{2}\omega_0-R_{aa}(E,\omega_0)][E+\tfrac{1}{2}\omega_0-\omega-R_{bb}(E,\omega_0)]-(\tfrac{1}{4}\omega_1)^2 = 0. \tag{6}$$

Solving this equation for every value of $\omega_0$, one gets $E$ as a function of $\omega_0$, ie the shape of the curve of figure 1. The extrema of the function $E = E(\omega_0)$ give the position of the centre of the resonance.

Differentiating equation (6) with respect to $\omega_0$ and putting $\mathrm{d}E/\mathrm{d}\omega_0 = 0$, one gets:

$$\begin{aligned}\left(\frac{1}{2}+\frac{\partial}{\partial\omega_0}R_{aa}(E,\omega_0)\right)[E+\tfrac{1}{2}\omega_0-\omega-R_{bb}(E,\omega_0)]\\ = \left(\frac{1}{2}-\frac{\partial}{\partial\omega_0}R_{bb}(E,\omega_0)\right)[E-\tfrac{1}{2}\omega_0-R_{aa}(E,\omega_0)].\end{aligned} \tag{7}$$

The two coordinates $E$ and $\omega_0$ of an extremum are solutions of the system of two equations (6) and (7). After some algebra, equations (6) and (7) are found to be equivalent to the following rigorous system:

$$\begin{cases} E = \tfrac{1}{2}\omega+\dfrac{1}{2}[R_{aa}(E,\omega_0)+R_{bb}(E,\omega_0)]+\tfrac{1}{4}\omega_1\left(Q(E,\omega_0)+\dfrac{1}{Q(E,\omega_0)}\right) & (8)\\ \omega_0 = \omega+R_{bb}(E,\omega_0)-R_{aa}(E,\omega_0)+\tfrac{1}{4}\omega_1\left(\dfrac{1}{Q(E,\omega_0)}-Q(E,\omega_0)\right) & (9)\end{cases}$$

where

$$Q = \left(\frac{1}{2}+\frac{\partial}{\partial\omega_0}R_{aa}\right)^{1/2}\left(\frac{1}{2}-\frac{\partial}{\partial\omega_0}R_{bb}\right)^{-1/2}. \tag{10}$$

Equations (8) and (9) give the coordinates of $A_1$. Those of $A_2$ are obtained by changing $Q$ into $-Q$. But symmetry considerations show that $A_1$ and $A_2$ have the same abscissa.

In order to obtain $\omega_0$ up to sixth order, we need the expression of $R_{aa}$ and $R_{bb}$ to the same order. It is then easy to solve equations (8) and (9) by iteration. We finally get:

$$\omega_0 = \omega-\frac{1}{\omega}(\tfrac{1}{4}\omega_1)^2-\frac{5}{4\omega^3}(\tfrac{1}{4}\omega_1)^4-\frac{61}{32\omega^5}(\tfrac{1}{4}\omega_1)^6. \tag{11}$$

In order to compare with Shirley's formula, which gives $\omega$ as a function of $\omega_0$, we need to inverse equation (11). Taking Shirley's notations ($b$ instead of $\tfrac{1}{4}\omega_1$), we obtain:

$$\omega = \omega_0+\frac{b^2}{\omega_0}+\frac{1}{4}\frac{b^4}{\omega_0{}^3}-\frac{35}{32}\frac{b^6}{\omega_0{}^5}. \tag{12}$$

This result exactly coincides with Shirley's expansion, and also with Pegg and Series' result.

Note that an experimental test of the higher order terms of expression (11) is not easy: when $\omega_1$ increases, the resonance is not only shifted, but also *broadened* and *distorted*, so that a precise determination of its centre becomes difficult.

Other kinds of magnetic resonance exist which are easier to study experimentally. We will show in the following letter how they can be used to check the theory given above.

## References


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