Black Body Radiation Shift of the $^{133}$Cs Hyperfine Transition Frequency

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Abstract

We report the theoretical evaluations of the static scalar polarizability of the $^{133}$Cs ground state and of the black body radiation shift induced on the transition frequency between the two hyperfine levels with $m_F = 0$. This shift is of fundamental importance in the evaluation of the accuracy of the primary frequency standards based on atomic fountains and employed in the realization of the SI second in the International Atomic Time (TAI) scale at the level of $1 \times 10^{-15}$.

Our computed value for the polarizability is $\alpha_0 = (6.600 \pm 0.016) \times 10^{-39} \text{Cm}^2/\text{V}$ in agreement at the level of $1 \times 10^{-3}$ with recent theoretical and experimental values. As regards the black body radiation shift we find for the relative hyperfine transition frequency $\beta = (-1.49 \pm 0.07) \times 10^{-14}$ at $T = 300$ K in agreement with frequency measurements reported by our group and by Bauch and Schröder [Phys. Rev. Lett. 78, 622, (1997)]. This value is lower by $2 \times 10^{-15}$ than that obtained with measurements based on the dc Stark shift and with the value commonly accepted up to now.

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I. Introduction

The evaluation of the accuracy of the cesium primary frequency standards requires to take into account, among others, the shift induced on the clock transition \( |6^2S_{1/2}, F = 4, m_F = 0 \rangle \rightarrow |6^2S_{1/2}, F = 3, m_F = 0 \rangle \) by the black body radiation (BBR). The definition of the second in the International System of Units (SI) is in fact based on the above transition observed in absence of any perturbation and then, in particular, at \( T = 0 \) K \[1\], where \( T \) is the temperature of the environment.

Gallagher and Cook \[2\] firstly considered the effects of BBR on the Rydberg states of the atoms while Itano et al. \[3\] focused their attention onto the atomic frequency standards. They reported the following expression for the relative frequency shift of the \(^{133}\text{Cs}\) clock transition \( (\nu_0 = 9192631770 \text{ Hz})\):

\[
\frac{\Delta \nu}{\nu_0} = \beta \left( \frac{T}{T_0} \right)^4 \left[ 1 + \epsilon \left( \frac{T}{T_0} \right)^2 \right]
\]

(1)

with \( \beta = -1.69(4) \times 10^{-14} \) and \( \epsilon = 1.4 \times 10^{-2} \) when \( T_0 = 300 \) K. This expression has been adopted till now to correct all the primary frequency standards for the BBR shift at an accuracy level of \( 10^{-15} \) or even better \[4\].

The BBR induces both non resonant ac Stark and Zeeman shifts of the atomic transitions. For the ground state \(^2S_{1/2}\) of the alkali-metal atoms the Zeeman shift is of the order of \( 10^{-17} \) \[3\] and is not relevant for the accuracy estimation of the present frequency standards.

The direct experimental method to evaluate the BBR shift is based on (1): the frequency shift \( \Delta \nu \) is measured versus the black body temperature \( T \) and the experimental points are fitted with (1) whose temperature dependence follows directly from the Planck radiation law. This method has been used by Bauch and Schroeder \[5\] employing a thermal cesium beam and in our group using an atomic fountain \[6\].

In order to increase the experimental resolution, the BBR shift may be also evaluated indirectly by measuring the dc Stark shift coefficient \( k \) defined as:

\[
\Delta \nu = kE^2
\]

(2)

where \( \Delta \nu \) is the frequency shift induced by the static electric field \( E \). Measurements of \( k \) have been performed in this way by Haun and Zacharias \[7\] and by Mowat \[8\], using a thermal beam and the Ramsey interrogation technique, and by Simon et al. \[9\] using an atomic fountain. The BBR shift is then obtained from (2) assuming \( E \):

\[
E^2 = \langle \mathcal{E}^2(t) \rangle = \frac{4\sigma T_0^4}{\varepsilon_0 c} \left( \frac{T}{T_0} \right)^4
\]

(3)

where \( \langle \mathcal{E}^2(t) \rangle \) is the mean-squared electric field of the black body radiation, \( \sigma = 5.670400(40) \times 10^{-8} \) W/m\(^2\)K\(^4\) is the Stefan-Boltzmann constant \[10\], \( \varepsilon_0 \) is the vacuum permittivity and \( c \) is
the speed of light in vacuum. In (3) the first identity is valid at a level of a few percent and can be corrected as reported in [3], while the second identity is obtained directly by the Planck radiation law (see next section).

The measurement of the scalar static polarizability $\alpha_0$ is related to the above method through the expression:

$$W = -\frac{1}{2}\alpha_0 E^2$$

(4)

where $W$ is the potential energy of a neutral atom in a static electric field $E$ of moderate strength.

Due to the very low intensity of the black body field, the hyperpolarizability effect is negligible and will not be considered throughout the paper.

The polarizability is obtained from the force acting on the atom when submitted to a gradient of the electric field:

$$F = -\nabla W = \alpha_0 E \nabla E$$

(5)

This force, in turn, can be measured through the deflection of thermal beams [12, 13], through E-H gradient balances [14, 15] or through the time of flight of cooled atoms in a fountain apparatus [16, 17]. In principle, the BBR shift can be also obtained from (3) and (4) as follows:

$$\Delta \nu = \frac{1}{\hbar} (W_\beta - W_\alpha) = -\frac{1}{2\hbar} \left[ \alpha_0(|\beta\rangle) - \alpha_0(|\alpha\rangle) \right] \langle E^2(t) \rangle$$

(6)

where $|\beta\rangle = |6^2S_{1/2}, F = 4, m_F = 0\rangle$ and $|\alpha\rangle = |6^2S_{1/2}, F = 3, m_F = 0\rangle$ in the Cs case; $\hbar$ is the Planck constant.

The indirect experimental technique allows a higher resolution, being possible to submit the atoms to dc fields of several MV/m, if compared to the black body field $\sqrt{\langle E^2(t) \rangle} = 832.2$ V/m at $T = 300$ K used in the direct method. Nevertheless, it is based on the conceptual assumption $E^2 = \langle E^2(t) \rangle$ and may not be free from spurious effects as we shall discuss further on.

From the theoretical point of view, the evaluation of the BBR shift requires the computation of the scalar polarizabilities of the two states defining the clock transition or, in other words, of the non resonant ac Stark shift. This is typically performed through perturbation techniques [18, 19]. More precisely, according to [20], we have to calculate the differential polarizability between the two ground state hyperfine levels. As pointed out by Feichtner et al. [20], this requires to consider in the theoretical analysis a basis of modified eigenfunctions which account for the hyperfine interaction of the ground and $P$ states with other states of the same quantum numbers $F$ and $m_F$. A review of the theoretical works leading to the evaluation of the ground state $^{133}$Cs polarizability can be found in [15] and in [17].

Due to the basic importance of the BBR shift correction to evaluate the present primary frequency standard accuracy at the $10^{-15}$ level and, in the next future at the $10^{-16}$ level, it is highly desirable to re-examine the relation (1) considering that:
(i) new and more precise experimental data are now available for the electric dipole moments and for the transition frequencies of $^{133}$Cs involved in the theoretical computation of $\alpha_0$;

(ii) recent theoretical evaluations of $\alpha_0$ [21] lead to a significantly lower value than that commonly assumed up to now [3, 8];

(iii) the two most precise measurements [9, 17] of the electrical polarizability do not agree to each other.

In this paper we report an ab-initio computation of the BBR shift for the clock transition which turns out lower by $2 \times 10^{-15}$ at 300 K than the commonly adopted value of [11]. A critical comparison with the theoretical and experimental values reported in the literature will be also given, showing the present difficulty to assess the accuracy at the $10^{-16}$ level for atomic frequency standards operating at $T \approx 300$ K.

II. Basic Theory

The non-resonant ac Stark shift $\Delta W^{(k)}_\alpha$ of the energy of state $|\alpha\rangle$ induced by the level $|k\rangle$ is given by [19]:

$$\Delta W^{(k)}_\alpha = \frac{|d_{\alpha k}|^2}{\hbar} \int_0^{+\infty} \frac{\nu_\alpha - \nu_k}{(\nu_\alpha - \nu_k)^2 - \nu^2} E^2_{\nu}(\nu) d\nu$$

(7)

where $d_{\alpha k} = e \langle \alpha | \mathbf{e} \cdot \mathbf{r} | k \rangle$ is the electric dipole moment of the transition $|k\rangle \rightarrow |\alpha\rangle$, $e$ the electron charge, $\mathbf{e}$ the polarization vector of the electric field, $\mathbf{r}$ the atomic position vector, $\nu_\alpha = W_\alpha/\hbar$ and $\nu_k = W_k/\hbar$ the energy levels of the states $|\alpha\rangle$ and $|k\rangle$ in frequency units and $E^2_{\nu}(\nu)$ the mean-squared value of the electric field at frequency $\nu$. When $|\alpha\rangle$ represents a ground state, we have $\nu_\alpha - \nu_k \equiv -\nu_{\alpha k} = -c/\lambda_{\alpha k}$ being $\nu_{\alpha k}$ and $\lambda_{\alpha k}$ the frequency and the wavelength of the atomic transition $|k\rangle \rightarrow |\alpha\rangle$. Figure 1 summarizes the above definitions. The electric field per frequency unit $E_{\nu}(\nu)$ is related to the spectral energy density $E_{\nu}(\nu, T)$ by the well known relation:

$$E_{\nu}(\nu, T) d\nu = \frac{1}{\varepsilon_0} E_{\nu}(\nu, T) d\nu$$

(8)

In our case the energy density $E_{\nu}(\nu, T) d\nu$ is given by the Planck radiation law:

$$E_{\nu}(\nu, T) d\nu = \frac{8\pi\hbar\nu^3}{c^3} \frac{d\nu}{e^{\hbar\nu/k_B T} - 1}$$

(9)

where $k_B$ is the Boltzmann constant.

The maximum of $E_{\nu}(\nu, T)$ is reached when (Wien law):

$$\nu = \nu_{\text{max}} = 2.821 \frac{k_B}{\hbar} T$$

(10)

At $T = 300$ K, relation (10) gives $\nu_{\text{max}} = 17.6$ THz. In the Cs case, the minimum value of $\nu_{\alpha k}$ corresponds to the D$_1$ optical transition (335 THz) so that $\nu_{\text{max}} \ll \nu_{\alpha k}$ for all $|k\rangle$ levels.
coupled to the state \( |\alpha\rangle \) and it is possible to omit the \( \nu^2 \) term in the denominator of (7) avoiding the singularity of the integrand at \( \nu = \nu_{ak} \). We shall consider further on the effect of this approximation. The basic relation (7) can then be written as:

\[
\Delta W_{\alpha}^{(k)} = -\frac{1}{\hbar} \frac{|d_{\alpha k}|^2}{\nu_{ak}} \langle \mathcal{E}^2(t) \rangle
\]  

(11)

where the mean-squared electric field \( \langle \mathcal{E}^2(t) \rangle \) is given by

\[
\langle \mathcal{E}^2(t) \rangle \equiv \int_0^{+\infty} \mathcal{E}_\nu^2(\nu) d\nu = \frac{4\sigma T^4}{\varepsilon_0 c}
\]  

(12)

The relation (12), obtained through (8) and (9), is also known as the Stefan-Boltzmann law; at \( T=300 \) K it gives \( \langle \mathcal{E}^2(t) \rangle = (832.2)^2 \) (V/m)^2, as already reported in the previous section.

Summing over all the excited states \( |k\rangle \) coupled to the level \( |\alpha\rangle \), we obtain the total Stark shift for the state \( |\alpha\rangle \):

\[
\Delta W_{\alpha} = -\frac{1}{\hbar} \sum_k \frac{|d_{\alpha k}|^2}{\nu_{ak}} \langle \mathcal{E}^2(t) \rangle
\]  

(13)

Moreover, taking (3) and (4) into account, it is possible to write (13) also in the following form:

\[
\Delta W_{\alpha} = -\frac{1}{2} \alpha_0 \langle \mathcal{E}^2(t) \rangle
\]  

(14)

where

\[
\alpha_0 = \frac{2}{\hbar} \sum_k \frac{|d_{\alpha k}|^2}{\nu_{ak}}
\]  

(15)

is the scalar polarizability of the state \( |\alpha\rangle \) which may be measured experimentally.

More precisely, the expression (15) takes into account the contribution to the polarizability from the valence excited states. In principle, the total polarizability includes also the contribution
from the core excited states \[22\]; however, this is not important for the clock transition shift since it is common to both the ground state sublevels.

The BBR shift \(\Delta \nu\) of the clock transition \(|\beta\rangle \rightarrow |\alpha\rangle\) we are looking for is:

\[
\Delta \nu = \frac{1}{\hbar} (\Delta W_\beta - \Delta W_\alpha)
\]  

(16)

Introducing relations (12) and (13) in (16) we finally obtain:

\[
\Delta \nu = \frac{4 \sigma T_0^4}{h^2 \varepsilon_0 c} \left( \frac{T}{T_0} \right)^4 \left\{ \sum_k \frac{|d_{\beta k}|^2}{\nu_\beta k} - \sum_k \frac{|d_{\alpha k}|^2}{\nu_\alpha k} \right\}
\]

\[
= \frac{2 \sigma T_0^4}{h^2 \varepsilon_0 c} \left( \frac{T}{T_0} \right)^4 \left\{ \alpha_0(|\beta\rangle) - \alpha_0(|\alpha\rangle) \right\}
\]  

(17)

We conclude this theoretical review observing that the dc Stark coefficient \(k\) defined in (2) can be expressed through the polarizabilities of the ground state levels (see also (6)) as:

\[
k = - \frac{1}{2h} \left\{ \alpha_0(|\beta\rangle) - \alpha_0(|\alpha\rangle) \right\} = - \frac{8 \alpha_{10}}{7 \hbar}
\]  

(18)

where \(\alpha_{10}\) is the scalar differential polarizability introduced by Sandars \[23\]. In the experimental measurement of \(k\) performed with a dc electric field a tensorial component is also present, which has to be subtracted in order to take the isotropy of the black-body radiation into account \[3, 9\].

III. Numerical Evaluation

To evaluate numerically the BBR shift given by (17) we need the matrix elements of the operator \(e \cdot r\); writing the atomic position vector \(r\) as an irreducible rank 1 tensor operator we have:

\[
e \cdot r = r_0 \cos \theta - \frac{1}{\sqrt{2}} r_1 \sin \theta e^{-i\varphi} + \frac{1}{\sqrt{2}} r_{-1} \sin \theta e^{i\varphi}
\]  

(19)

where \(r\) is expressed in terms of its spherical components \(r_0, r_{-1}\) and \(r_1\); \(\theta\) (co-latitude) and \(\varphi\) (azimuth) are the polar angles defining the electric field direction with respect to the quantization axis (z axis). The well-known Wigner-Eckart \[24\] theorem allows us to simplify the generic matrix element:

\[
\langle 6S_{1/2}; F, m_F | e r_q | n' P_{J'} F', m_{F'} \rangle = Q(F, m_F; F', m_{F'}; J, J'; q) \langle 6S_{1/2} || e r || n' P_{J'} \rangle
\]  

(20)

where the double bars indicate the dipole reduced matrix element and \(q\) is the index labelling the component of \(r\). In (20) we defined:

\[
Q(F, m_F; F', m_{F'}; J, J'; q) \equiv (-1)^{F-m_F+F'+J+I+1} \sqrt{(2F+1)(2F'+1)}
\]

\[
\times \begin{pmatrix}
F & 1 & F' \\
-m_F & q & m'_{F'}
\end{pmatrix}
\begin{pmatrix}
F & 1 & F' \\
J' & I & J
\end{pmatrix}
\]  

(21)
where the coefficients in round and in curly brackets are the 3-$j$ and 6-$j$ symbols respectively. The primed quantum numbers refer to the excited states $|n'P_J'$) coupled to the ground state by allowed electric dipole transitions.

The polarizability of each of the two ground state levels can then be written as:

$$
\alpha_0(|F, m_F) = \frac{2}{4\pi \hbar} \int d\Omega \sum_{n' \geq 6, J', F', m'_F} \left| \left( \frac{6S_{1/2}}{\nu(6S_{1/2} \rightarrow 6P_{J'})} \right) Q(F, m_F; F', m'_F; J, J'; q = 0) \cos \theta - \frac{1}{\sqrt{2}} Q(F, m_F; F', m'_F; J, J'; q = 1) \sin \theta e^{-i\varphi} + \frac{1}{\sqrt{2}} Q(F, m_F; F', m'_F; J, J'; q = -1) \sin \theta e^{i\varphi} \right|^2
$$

(22)

In [22] we perform an integration over the solid angle $\Omega$ to take the isotropic nature of the BBR into account, consequently the integral is normalized to $4\pi$; $\nu(6S_{1/2} \rightarrow 6P_{J'})$ is the frequency of the transition indicated in parentheses. According to selection rules, for fixed values of the quantum numbers only one of the three $Q$ terms is not zero.

Actually, as Feichtner et al. [20] pointed out, the $S_{1/2}$ state and the $P$ states wave functions are perturbed by the effect of their hyperfine interaction with other states with the same $F$ and $m_F$ but with different principal quantum number $n$. Therefore, the dipole matrix elements should not be calculated between the unperturbed wave functions but between the perturbed ones defined as:

$$
\langle 6S_{1/2}; F \rangle \equiv \langle 6S_{1/2}; F \rangle + \sum_{n = 7}^{\infty} a_{nF} \langle nS_{1/2}; F \rangle
$$

(23)

$$
\langle 6P_{J'}; F' \rangle \equiv \langle 6P_{J'}; F' \rangle + \sum_{n = 7}^{\infty} b_{nJ'F'} \langle nP_{J'}; F' \rangle
$$

$$
\langle 7P_{J'}; F' \rangle \equiv \langle 7P_{J'}; F' \rangle + \sum_{\substack{n = 6 \ n \neq 7}} c_{nJ'F'} \langle nP_{J'}; F' \rangle
$$

The coefficients $a_{nF}$, $b_{nJ'F'}$ and $c_{nJ'F'}$, given in [20], are here reported for convenience.

$$
\begin{align*}
a_{nJF} &= \left( \frac{\psi_{nS}}{\psi_{6S}} \right) \left[ \frac{33}{8} - F(F + 1) \right] \left[ \frac{\nu_0}{\nu(nS_{1/2} \rightarrow 6S_{1/2})} \right] \\
b_{nJF} &= \left( \frac{\psi_{nS}}{\psi_{6S}} \right) \left[ \frac{63}{32J(J + 1)} - F(F + 1) \right] \left[ \frac{\nu_0}{\nu(nP_J \rightarrow 6P_J)} \right] \\
c_{nJF} &= \left( \frac{\psi_{7S}}{\psi_{6S}} \right)^2 \left[ \frac{63}{32J(J + 1)} - F(F + 1) \right] \left[ \frac{\nu_0}{\nu(nP_J \rightarrow 7P_J)} \right]
\end{align*}
$$

(24)

and their numerical values are reported in Tables 1, 2 and 3.
Table 1: Coefficients $a_{nJF}$ (in units of $10^{-6}$) for perturbed cesium $6S$ wave function.

| $n$ | $J\backslash F$ | 4   | 3   |
|-----|-----------------|-----|-----|
| 7   | 1/2             | -3.37 | +4.33 |
| 8   | 1/2             | -1.63 | +2.08 |
| 9   | 1/2             | -1.04 | +1.34 |

Table 2: Coefficients $b_{nJF}$ (in units of $10^{-6}$) for perturbed cesium $6P$ wave function.

| $n$ | $J\backslash F$ | 5           | 4   | 3   | 2   |
|-----|-----------------|--------------|-----|-----|-----|
| 7   | 1/2             | -1.966       | +2.529 | \   |
| 8   | 1/2             | -0.904       | +1.16 | \   |
| 9   | 1/2             | -0.567       | +0.729 | \   |
| 7   | 3/2             | -1.223       | -0.0583 | +0.874 | +1.573 |
| 8   | 3/2             | -0.560       | -0.026 | +0.400 | +0.721 |
| 9   | 3/2             | -0.351       | -0.017 | +0.250 | +0.452 |

Table 3: Coefficients $c_{nJF}$ (in units of $10^{-6}$) for perturbed cesium $7P$ wave function

| $n$ | $J\backslash F$ | 5           | 4   | 3   | 2   |
|-----|-----------------|--------------|-----|-----|-----|
| 6   | 1/2             | +1.966       | -2.529 | \   |
| 8   | 1/2             | -1.539       | +1.980 | \   |
| 9   | 1/2             | -0.741       | +0.953 | \   |
| 6   | 3/2             | +1.223       | +0.0583 | -0.874 | -1.573 |
| 8   | 3/2             | -0.957       | -0.0455 | +0.684 | +1.230 |
| 9   | 3/2             | -0.455       | -0.0217 | +0.325 | +0.585 |

These coefficients are very small (of the order of $10^{-6}$) and their contribution to the absolute value of the scalar polarizability is completely negligible. However, they must be taken into account in order to obtain the correct value of the differential polarizability we are interested in.

The ground state wave function is more sensitive to the hyperfine interaction so in this calculation the corresponding sum in (23) has been extended from $n = 7$ to $n = 9$; the coefficients $b_{nJF}$ and $c_{nJF}$ essentially involve higher order corrections and we considered only the first term.
in the respective perturbative sums.

As an example, we report in the following equation the expression of the polarizability of the level \(|6S_{1/2}; F = 4, m_F = 0\) due only to the interaction with the excited level \(|6P_{1/2}\):

\[
\alpha_0(|F = 4, m_F = 0\rangle) = \frac{2}{4\pi\hbar} \int \frac{d\Omega}{4\pi} \sum_{F', m'_F} \left[ Q(4, 0; F', m'_F; 1/2, 1/2; q = 0) \cos \theta - \frac{1}{\sqrt{2}} Q(4, 0; F', m'_F; 1/2, 1/2; q = 1) \sin \theta e^{-i\phi} + \frac{1}{\sqrt{2}} Q(4, 0; F', m'_F; 1/2, 1/2; q = -1) \sin \theta e^{i\phi} \right]^2 \\
\times \frac{1}{\nu(6S_{1/2} \rightarrow 6P_{1/2}; F')} \left[ 6S_{1/2} |er||6P_{1/2} \rangle + \sum_{n=7}^{9} a_{n\frac{3}{2}4} \langle nS_{1/2}|er||6P_{1/2} \rangle + b_{7\frac{3}{2}F'} \langle 6S_{1/2}|er||7P_{1/2} \rangle + \sum_{n=7}^{9} a_{n\frac{1}{2}4} b_{7\frac{1}{2}F'} \langle nS_{1/2}|er||7P_{1/2} \rangle \right]^2
\]

(25)

For both the ground-state hyperfine levels, we calculated similar contributions due to the excited states \(|6P_{3/2}, 7P_{1/2}, 7P_{3/2}, 8P_{1/2}, 8P_{3/2}\). In the case of \(|6P_{1/2}\) and \(|6P_{3/2}\) (D1 and D2 line, respectively), we also included their hyperfine structure [25].

To evaluate numerically the absolute and the differential polarizability we need to know the reduced dipole matrix elements and the frequencies of the transitions involved in this calculation. Several experimental [17, 20, 27, 28] and theoretical [29, 30, 31, 32] works have been devoted to the determination of the dipole matrix elements. In particular, the measurement of the excited states \(|6P_{1/2}\) and \(|6P_{3/2}\) lifetimes provides a direct method to know the reduced matrix elements through the well-known expression of the spontaneous emission:

\[
\frac{1}{\tau_{J'}} = \frac{\omega_{nk}^3}{3\pi c \varepsilon_0 \hbar c^3} \frac{1}{2J' + 1} |\langle 6^2 S_{1/2}|er||6^2 P_{J'} \rangle|^2
\]

(26)

being \(\tau_{J'}\) the lifetime of the transition \(|k \rightarrow |a\rangle\). For D1 and D2 lines, performing an average of the lifetimes reported in Table 2 of [17] we obtain: \(\tau_{1/2} = (34.86 \pm 0.05)\) ns and \(\tau_{3/2} = (30.44 \pm 0.04)\) ns. However, due to the dispersion of these values we considered an error bar that is twice the calculated one. For the reduced dipole moments \(\langle 6S_{1/2}|er||nP_{J} \rangle (n=7,8), \langle 7S_{1/2}|er||7P_{J} \rangle \) and \(\langle 6P_{J}|er||7S_{1/2} \rangle\) we perform an average over the theoretical and experimental values reported in Table 6 of [30]. For the matrix elements \(\langle 7S_{1/2}|er||8P_{J} \rangle\) we use the values of [32] to whom we attribute an uncertainty of the 1%. The signs of the matrix elements are chosen according to the Feichtner et al. paper. All the values of the dipole matrix elements used in this numerical evaluation are summarized in Table 4.

In Table 5, we report the values of the atomic transitions frequencies we use. For the frequencies of D1 and D2 lines we use the most accurate values presently available [25]. For the other transitions we use the values reported in the Basic Atomic Spectroscopic Database of NIST.
Table 4: Reduced dipole matrix elements of the atomic transitions used in this calculation.

| Dipole Matrix Element | Value in $10^{-29}$ C·m |
|-----------------------|--------------------------|
| $\langle 6S_{1/2}\|er\|6P_{1/2}\rangle$ | -3.8174(56)$^a$ |
| $\langle 6S_{1/2}\|er\|6P_{3/2}\rangle$ | -5.3729(70)$^a$ |
| $\langle 6S_{1/2}\|er\|7P_{1/2}\rangle$ | 0.237(4)$^b$ |
| $\langle 6S_{1/2}\|er\|7P_{3/2}\rangle$ | 0.491(3)$^b$ |
| $\langle 6P_{1/2}\|er\|7S_{1/2}\rangle$ | 3.59(1)$^b$ |
| $\langle 6P_{3/2}\|er\|7S_{1/2}\rangle$ | 5.487(8)$^b$ |
| $\langle 7S_{1/2}\|er\|7P_{1/2}\rangle$ | -8.71(11)$^b$ |
| $\langle 7S_{1/2}\|er\|7P_{3/2}\rangle$ | -12.11(1)$^b$ |
| $\langle 6P_{1/2}\|er\|8S_{1/2}\rangle$ | -0.85(9)$^d$ |
| $\langle 6P_{3/2}\|er\|8S_{1/2}\rangle$ | -1.23(12)$^d$ |
| $\langle 6S_{1/2}\|er\|8P_{1/2}\rangle$ | -0.066(2)$^b$ |
| $\langle 6S_{1/2}\|er\|8P_{3/2}\rangle$ | -0.183(2)$^b$ |
| $\langle 7S_{1/2}\|er\|8P_{1/2}\rangle$ | 0.776(1)$^c$ |
| $\langle 7S_{1/2}\|er\|8P_{3/2}\rangle$ | 1.374(14)$^c$ |
| $\langle 7P_{1/2}\|er\|8S_{1/2}\rangle$ | 7.41(70)$^d$ |
| $\langle 7P_{3/2}\|er\|8S_{1/2}\rangle$ | 11.5(1)$^d$ |
| $\langle 6P_{1/2}\|er\|9S_{1/2}\rangle$ | 0.46(5)$^d$ |
| $\langle 6P_{3/2}\|er\|9S_{1/2}\rangle$ | 0.65(6)$^d$ |
| $\langle 7P_{1/2}\|er\|9S_{1/2}\rangle$ | -1.67(17)$^d$ |
| $\langle 7P_{3/2}\|er\|9S_{1/2}\rangle$ | -2.2(2)$^d$ |

$^a$ see text

$^b$ from Ref. [30]

$^c$ from Ref. [32]

$^d$ from Ref. [20]
Table 5: Frequencies of the atomic transitions used in this calculation.

| Transition                          | Frequency (THz) |
|-------------------------------------|-----------------|
| $|6S_{1/2}; F = 4\rangle \rightarrow |6P_{1/2}; F' = 3\rangle$ | 335.1113702     |
| $|6S_{1/2}; F = 4\rangle \rightarrow |6P_{1/2}; F' = 4\rangle$ | 335.1125378     |
| $|6S_{1/2}; F = 4\rangle \rightarrow |6P_{3/2}; F' = 3\rangle$ | 351.7215083     |
| $|6S_{1/2}; F = 4\rangle \rightarrow |6P_{3/2}; F' = 4\rangle$ | 351.7217095     |
| $|6S_{1/2}; F = 4\rangle \rightarrow |6P_{3/2}; F' = 5\rangle$ | 351.7219605     |
| $|6S_{1/2}; F = 4\rangle \rightarrow |7P_{1/2}\rangle$       | 652.50476       |
| $|6S_{1/2}; F = 4\rangle \rightarrow |7P_{3/2}\rangle$       | 657.93238       |
| $|6S_{1/2}; F = 4\rangle \rightarrow |8P_{1/2}\rangle$       | 770.73660       |
| $|6S_{1/2}; F = 4\rangle \rightarrow |8P_{3/2}\rangle$       | 773.21409       |
| $|6S_{1/2}; F = 3\rangle \rightarrow |6P_{1/2}; F' = 3\rangle$ | 335.1205628     |
| $|6S_{1/2}; F = 3\rangle \rightarrow |6P_{1/2}; F' = 4\rangle$ | 335.1217305     |
| $|6S_{1/2}; F = 3\rangle \rightarrow |6P_{3/2}; F' = 2\rangle$ | 351.7305497     |
| $|6S_{1/2}; F = 3\rangle \rightarrow |6P_{3/2}; F' = 3\rangle$ | 351.7307010     |
| $|6S_{1/2}; F = 3\rangle \rightarrow |6P_{3/2}; F' = 4\rangle$ | 351.7309021     |
| $|6S_{1/2}; F = 3\rangle \rightarrow |7P_{1/2}\rangle$       | 652.51395       |
| $|6S_{1/2}; F = 3\rangle \rightarrow |7P_{3/2}\rangle$       | 657.94157       |
| $|6S_{1/2}; F = 3\rangle \rightarrow |8P_{1/2}\rangle$       | 770.74579       |
| $|6S_{1/2}; F = 3\rangle \rightarrow |8P_{3/2}\rangle$       | 773.22328       |

These frequencies are known with an accuracy high enough so that we do not consider their contribution to the evaluation of the uncertainty in the final result.

As far as the $a_{nJF}$, $b_{nJF}$ and $c_{nJF}$ coefficients are concerned, we observe that in their definition the knowledge of the wave function at the origin is required. In turn, the wave function depends on the potential used to describe the interaction of the valence electron with the nucleus and with the closed electron shells [33]. In other words, this potential accounts for the departure from the hydrogen potential. Due to the difficulty in modelling this interaction, we made a conservative estimation, attributing an uncertainty of 10% to the coefficients $a_{nJF}$, $b_{nJF}$ and $c_{nJF}$.

Inserting all these quantities and the respective uncertainties in (17) we obtain:

$$\frac{\Delta \nu}{\nu_0} = (-1.49 \pm 0.07) \times 10^{-14} \left(\frac{T}{T_0}\right)^4$$  \hspace{1cm} (27)

In (27) the uncertainty is mainly due to the uncertainty of the coefficients $a_{nJF}$, $b_{nJF}$ and $c_{nJF}$.

We notice that the result (27) has been obtained by means of the integration in (22) over the
solid angle $\Omega$ which has allowed us to calculate the scalar polarizability we are interested in; as a check, we obtain the same value using directly the Sandars formula \[23\]. If we estimate the BBR shift by using the polarizability value computed for a well defined orientation of the electric field with respect to the quantization axis, the non-zero tensorial part of the polarizability itself leads to small errors in the coefficient $\beta$. More precisely, $\beta$ changes of about $3 \times 10^{-16}$ in $^{133}\text{Cs}$, depending on whether the electric field is parallel or perpendicular to the $z$ axis.

From \[17\] and \[18\] we have also for the Stark shift coefficient:

$$k = -(1.97 \pm 0.09) \times 10^{-10} \text{ Hz/(V/m)}^2$$ (28)

and for the differential polarizability:

$$\alpha_{10} = (1.14 \pm 0.05) \times 10^{-43} \text{ J/(V/m)}^2$$ (29)

Moreover, our computations give for the scalar polarizability $\alpha_0^v$ of the $6^2S_{1/2}$ state of $^{133}\text{Cs}$ due only to the valence states:

$$\alpha_0^v = (6.341 \pm 0.016) \times 10^{-39} \text{ Cm}^2/\text{V}$$

$$= (56.99 \pm 0.14) \times 10^{-24} \text{ cm}^3$$ (30)

$$= (384.9 \pm 0.9)a_0^3$$

In \[30\] the first result is the value expressed in SI units, the second one in CGS units and the third one in atomic units, being $a_0$ the Bohr radius.

Finally, our evaluation of the corrective term $\epsilon$ is (see Appendix):

$$\epsilon = 1.4 \times 10^{-2}$$

in agreement with the value reported in \[3\].

IV. Discussion of the results

We firstly examine the scalar polarizability value reported in \[30\]; even if it does not lead directly to the BBR shift of the hyperfine transition we are looking for, it represents anyway an important check of a part of our computations and provides an independent estimation of this important parameter. The total scalar polarizability $\alpha_0$ must take the core polarizability $\alpha_0^c$ into consideration which accounts for approximately the 4 % of the total value in the case of $^{133}\text{Cs}$ \[22\]. Our final result for $\alpha_0$ is then:

$$\alpha_0 = \alpha_0^v + \alpha_0^c = (6.600 \pm 0.016) \times 10^{-39} \text{ Cm}^2/\text{V}$$

$$=(59.32 \pm 0.14) \times 10^{-24} \text{ cm}^3$$ (31)

$$=(400.7 \pm 1.0)a_0^3$$
Table 6: Cesium ground state polarizability.

| $\alpha_0 \times 10^{-39} \text{ Cm}^2/\text{V}$ | Reference                  |
|---------------------------------|---------------------------|
| 6.587 ± 0.031                  | Derevianko et al. [22]    |
| 6.596 ± 0.013                  | Derevianko and Porsev [21]|
| 6.600 ± 0.016                  | this work                 |
| 6.611 ± 0.009                  | Amini et al. [17]         |

where $\alpha_0^v$ is given by [30] and $\alpha_0^c$ is reported in [30].

In Table 6 we report the data found in literature with an uncertainty lower than 1 %.

An agreement at a level of $\pm 1 \times 10^{-3}$ can be observed, well inside the quoted error bars, both between the theoretical computations and with respect to the experimental value of Amini and Gould [17].

In Figure 2 the result of our computations concerning the BBR shift parameter $\beta$ is compared with the experimental results reported in literature.

Our result agrees with the direct measured values while the indirect measurements, even if in agreement among them, are higher by three standard deviations. This discrepancy has to be deeply examined not only for the correct estimation of the differential polarizability of the ground state hyperfine transition but also for its impact into the accuracy evaluation of the primary frequency standards. First of all, the following points have to be considered:

(i) our theoretical result leads to a polarizability $\alpha_0$ of the $^2S_{1/2}$ state in agreement with the most recent and precise evaluations as shown in Table 6, while the indirect measurements, considering that the Stark effect is proportional to the polarizability at the first order, lead to a considerably higher value for $\alpha_0$;

(ii) our computations lead to the result of Itano et al. [3] if we use the old values of the transition frequencies [34] and of the electric dipole moments [20, 33]; the latter, in particular, are considerably higher than the most precise recent values;

(iii) our $\beta$ value agrees with the values obtained with the direct measurement method.

Taking the above remarks into account, the following hypothesis may be considered in order to explain this discrepancy:

(i) the assumption of equivalence between ac and dc Stark shifts is not fully correct, in spite also of the correction term $\epsilon$ introduced by Itano et al. [3];
(ii) a systematic shift is present in the indirect measurements due to a physical effect not considered and present in the experiment.

Since we have no reason at the moment to believe in the breakdown of the equivalence between ac and dc Stark shifts, as far as the second hypothesis is concerned, the following point should be examined. All the measurements performed with the indirect method are based on a Ramsey interaction scheme with a Stark field applied during the free flight of the atoms between the two interaction regions. The atoms experience then two sudden changes of the electric field which could perturb the free evolution of the hyperfine coherence or induce Majorana-type transitions.

The last hypotheses must be considered more a clue than a probe to explain the discrepancy under question and obviously requires a more complete theoretical treatment.

V. Conclusions

We have reported in this paper a theoretical evaluation of the $^2S_{1/2}$ ground state polarizability of $^{133}$Cs and the BBR shift of the ground state hyperfine transition between the magnetic field independent sublevels. The former is in really good agreement with recent theoretical and experimental values; the latter agrees with the direct measurements reported in the literature and is lower by three standard deviations than the values obtained from dc Stark measurements.
The discrepancy of $2 \times 10^{-15}$ at $T=300$ K between the more recent estimations and the value accepted up to now impacts the accuracy evaluation of the primary frequency standards at the level of two or three times their believed standard uncertainties. Moreover, serious problems may be expected from the BBR shift to assess the accuracy at the level of $1 \times 10^{-16}$ for the future microwave frequency standards operating at $T \sim 300$ K.

Appendix

To avoid the singularity at $\nu = \nu_{\alpha k}$ in section II we have omitted the $\nu^2$ term in the denominator of (7). This simplification, usually adopted in literature, is justified by the fact that near room temperature the energy content of the BBR is peaked at frequencies much lower than the lowest transition frequency of the atom. An estimation of the error due to this approximation is provided in [3] with the introduction of the corrective term $\epsilon$ in (11). Here we re-evaluate this term following also the method described in [35].

Relations (7), (8) and (9) give:

$$\Delta W^{(k)} = -\frac{8\pi |d_{\alpha k}|^2 \nu_{\alpha k}}{\varepsilon_0 c^3} \left( \frac{k_B T}{\hbar} \right)^2 \sum_{n=1}^{\infty} \int_0^{+\infty} \frac{1}{1 - \frac{x^2}{\gamma_{\alpha k}^2}} \frac{x^3 dx}{e^x - 1}$$  \hspace{1cm} (32)

where $\gamma_{\alpha k} = \frac{\hbar \nu_{\alpha k}}{k_B T} \gg 1$ and $x = \frac{\hbar \nu_{\alpha k}}{k_B T}$. Expanding in (32) the factor:

$$\frac{1}{1 - \frac{x^2}{\gamma_{\alpha k}^2}} \approx 1 + \frac{x^2}{\gamma_{\alpha k}^2} + \frac{x^4}{\gamma_{\alpha k}^4} + ...$$  \hspace{1cm} (33)

and integrating we obtain:

$$\Delta W^{(k)} = -\frac{8\pi |d_{\alpha k}|^2 \nu_{\alpha k}}{\varepsilon_0 c^3} \left( \frac{k_B T}{\hbar} \right)^2 \sum_{n=1}^{\infty} \left( \frac{k_B T}{\hbar \nu_{\alpha k}} \right)^{2n} \frac{(2\pi)^{2n+2} |B_{2n+2}|}{4(n+1)}$$  \hspace{1cm} (34)

being $B_n$ the Bernoulli numbers. If we consider the main ($n = 1$) and the first order ($n = 2$) terms of (34) and sum over all the valence states, we obtain:

$$\Delta W_{\alpha} = -\frac{4\sigma T^4}{\hbar \varepsilon_0 c} \left( \frac{T}{T_0} \right)^4 \sum_k \frac{|d_{\alpha k}|^2}{\nu_{\alpha k}} \left\{ 1 + \frac{40\pi^2}{21} \left( \frac{k T_0}{\hbar \nu_{\alpha k}} \right)^2 \left( \frac{T}{T_0} \right)^2 \right\}$$  \hspace{1cm} (35)

We substitute now (35) in (16) and after some algebraic arrangements we obtain:

$$\Delta \nu = -\frac{4\sigma T^4}{\hbar^2 \varepsilon_0 c} \left( \frac{T}{T_0} \right)^4 \left\{ \sum_k \frac{|d_{\beta k}|^2}{\nu_{\beta k}} - \sum_k \frac{|d_{\alpha k}|^2}{\nu_{\alpha k}} \right\} \left[ 1 + \epsilon \left( \frac{T}{T_0} \right)^2 \right]$$  \hspace{1cm} (36)

where

$$\epsilon = \frac{40\pi^2}{21} \left( \frac{k_B T_0}{\hbar} \right)^2 \frac{\sum_k |d_{\beta k}|^2}{\nu_{\beta k}^2} - \frac{\sum_k |d_{\alpha k}|^2}{\nu_{\alpha k}^2} - \frac{\sum_k |d_{\alpha k}|^2}{\nu_{\beta k}^2} - \frac{\sum_k |d_{\beta k}|^2}{\nu_{\alpha k}^2}$$  \hspace{1cm} (37)
The main term of (36) coincides with (17), as expected. As regards the corrective term $\epsilon$, following the same procedure to evaluate the dipole matrix elements in the basis of modified eigenfunctions as reported in section III, we obtain $\epsilon = 1.4 \times 10^{-2}$, in agreement with the value reported in [3]. This agreement is not surprising because the recent values of the the dipole moments affect significantly the main parameter $\beta$, but much less the corrective term $\epsilon$, as can be observed in (37) where they appear both in the numerator and in the denominator.

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