Metrologia **43** (2006) L11–L13 doi:10.1088/0026-1394/43/3/N02

SHORT COMMUNICATION

Comment on ‘Evaluation of the primary frequency standard NPL-CsF1’*

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Received 20 June 2005
Published 21 February 2006

Abstract
A recent evaluation of the accuracy of the National Physical Laboratory (NPL) primary frequency standard NPL-CsF1 by K Szymaniec *et al* (2005 *Metrologia* **42** 49–57) reported an overall frequency uncertainty of $\delta\nu/\nu_0 = 1 \times 10^{-15}$. This stated uncertainty includes a correction of a frequency bias of $\delta\nu/\nu_0 = 8 \times 10^{-16} \pm 3 \times 10^{-16}$ attributed by the authors to microwave leakage. We believe that the stated cause of the frequency bias, its magnitude and its stated uncertainty are in error.

In their paper [1] on page 55, section 3.4 the authors state that a frequency shift in the National Physical Laboratory (NPL)-CsF1 primary frequency standard induced by microwave leakage is linearly dependent on microwave power. However, several studies and models have demonstrated that the magnitude of the frequency shift caused by microwave leakage is a power series in the microwave *field* with a leading term linear in the field [2–4]. The frequency shift due to microwave leakage at a Ramsey excitation of, for example, $11\pi/2$ would have a magnitude approximately 11 times the magnitude of the shift at $\pi/2$ rather than the factor of $11^2 = 121$ assumed in [1].

The paper reporting the evaluation of NPL-CsF1 [1] did not include detailed data on the measured frequency shift as a function of microwave power. However, an earlier paper about NPL-CsF1 [5] included data which appear to be consistent with a quasi-linear relationship between frequency shift and microwave power. The data from [5] are reproduced in figure 1. Both the reported frequency bias and associated uncertainty assigned to microwave leakage in [5] are identical to those reported in the formal evaluation of NPL-CsF1 [1].

The data in figure 1 are used to support the claimed strictly linear dependence of frequency shift on microwave power. We question this claim for several reasons. First, the uncertainty bars on the data in figure 1 average more than $\delta\nu/\nu = 10^{-14}$, some 30 times the claimed accuracy of the corrected frequency bias. These data are too crude, in and of themselves, to justify a correction of a primary frequency standard at the $\delta\nu/\nu \approx 3 \times 10^{-16}$ level based on an assumed strict linearity between microwave power and frequency shift. Second, the data in figure 1 can also be fitted with terms proportional to the microwave field amplitude (as suggested by theory), in addition to the term assumed to be linear in the microwave power. If these terms proportional to the field are included, the frequency bias at normal power would be shifted by $\delta\nu/\nu \approx 3.5 \times 10^{-15}$, more than ten times the claimed uncertainty of the bias and more than three times the *total* claimed uncertainty of the standard.

We note that in all previous reports of frequency bias caused by microwave leakage in fountain frequency standards, measurements of the sort shown in figure 1 have always been null-shift measurements; that is, they are used to evaluate the uncertainty of an uncorrected bias, not to make a correction for a bias. This is because microwave leakage is often unstable in time and corrections are thus difficult at best.

The authors at NPL state they have based their approach on a non-resonant AC Stark shift theory [6] and invoke the paper by Boussert *et al* [3] as justification. The frequency shift assigned is thus given as

$$\delta\nu \propto \frac{b_p^2}{2kv}, \qquad (1)$$

where kv is the detuning caused by the Doppler shift and b_p is the Rabi frequency associated with the leakage. The assumed strict linearity between microwave power and frequency shift is thus based on equation (1) in analogy with the light shift. The claim is made that the condition for large detuning is $kv \gg b_p$ and that within the large detuning limit only equation (1) is

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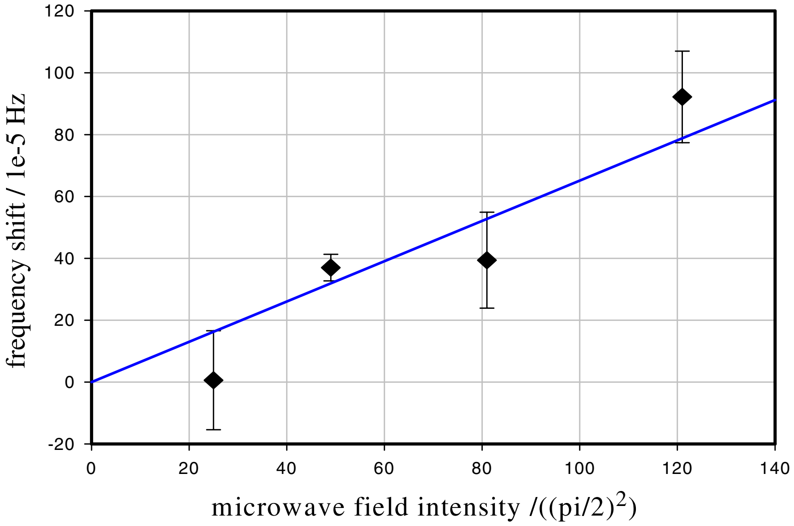

Figure 1. This is figure 8 of [5], along with the original figure caption: frequency difference NPL-CsF1-HM3 measured for microwave intensities corresponding to 5, 7, 9, $11\pi/2$ pulses experienced by atoms in the Ramsey cavity.

needed to account for the frequency shift caused by microwave leakage. The authors take $v \leqslant 2\,\mathrm{mm\,s^{-1}}$, which corresponds to a Doppler shift of some 0.060 Hz, and state that within their fountain $b_\mathrm{p}/b_0 \sim 10^{-5}$ (which implies that $b_\mathrm{p} \approx 1 \times 10^{-3}\,\mathrm{s^{-1}}$ at optimum power). In other words a leakage field well within the Ramsey fringe can be considered 'far from resonance'. Both the work of Boussert, in the large Doppler limit [3], and our own work in the small Doppler limit [4, 7] reach the conclusion that equation (1) is insufficient to describe the frequency shift caused by detuning and that in both the cases the shift is generally proportional to the amplitude of the leakage. This strongly suggests that the large detuning limit is not set by the Doppler shift as claimed by the authors of [1]. We further note that the light shift theory was developed for the case where the 'leakage' field frequency is much larger than the hyperfine splitting and generally couples both hyperfine states to a third excited state. Here the leakage field directly couples the two hyperfine states to each other, a different case altogether.

Boussert *et al* in [3] carefully analyse frequency shifts in thermal beam style caesium frequency standards in the large Doppler detuning limit (the case claimed to apply to the NPL standard) and clearly show that the frequency shift formulae contain terms linear in the microwave field amplitude that are, in general, larger than the quadratic term in equation (1).

This is further explored by Boussert *et al* [3]. In that reference, results which contain (1) are given as equations (43) and (44), reproduced below:

$$\Omega_\mathrm{r} = [(1/T)(b_\mathrm{p}/kv)(\cos^2(kL/2) - (\sin kL/kL))F - (1/T)(b_\mathrm{p}^2/2kv)H]\left[\int 2T^2 \sin b\tau(\sin b\tau(\tfrac{1}{4} + 1/(b\tau)^2) + (2/bT)\sin^2(b\tau/2))f(\tau)\,\mathrm{d}\tau\right]^{-1} (43) \qquad (2)$$

when $\Phi = 0$ and

$$\Omega_\mathrm{r} = \frac{(1/T)(b_\mathrm{p}/kv)\sin^2(kL/2)G - (1/T)(b_\mathrm{p}^2/2kv)H}{\int(T^2/2)(\sin b\tau + (4/bT)\sin^2(b\tau/2))^2 f(\tau)\,\mathrm{d}\tau} (44) \qquad (3)$$

when $\Phi = \pi$. Here Φ is the phase of the leakage field. We have taken the liberty in equations (2) and (3) of replacing the length of the Ramsey cavity, L, by vT, where v is the average atomic velocity and T is the Ramsey time, in order to clearly illustrate the terms of order b_p/kv and b_p^2/kv. Here Ω_r is the frequency shift and F, G and H are weighting functions which are unrelated to the size of the microwave leakage field. F and G are proportional to $\cos(b\tau)$ and so may be quite small around optimum power. However, using reasonable numbers for a caesium fountain ($T = 0.5$ s, $\tau = 0.01$ s, $b \sim 157$) along with a mono-velocity atomic distribution and the leakage amplitude claimed for the NPL fountain ($b_\mathrm{p}/b_0 \approx 10^{-5}$), suggests that optimum power must be set correctly at greater than the -100 dB level in order to neglect the first order term in equations (2) or (3) while retaining the second order term. No existing caesium fountain can claim to set optimum power at anything approaching this level and, indeed, the required stability of the microwave power is at or beyond the current state of the art. For example, in NIST-F1 we generally are quite careful in setting optimum power and struggle to set optimum microwave power to better than 1% (-20 dB).

The point is that the frequency shift given by (2) and (3) is a power series in the *amplitude* of the leakage field, b_p. The NPL group has taken only the second order term in b_p while neglecting completely the first order term, which is generally more important. While it is theoretically possible to arrange things so that the first order term is, in fact, zero it is highly unlikely (and would require microwave power stability beyond the state of the art) and would, in any case, be extremely difficult to prove in practice. The proof of the absolute vanishing of the linear term is required before the approach of NPL can be considered valid. To quote from Boussert *et al*:

> *There are two contributions at the lowest orders of perturbation because in this derivation we kept terms in* $b_\mathrm{p}^2/2kv$.

(as well as the term linear in b_p).

They continue

> *This contribution, which was neglected in (36) and (37) may here be of the same order of magnitude due to the presence of the small factor* $\cos(b\tau)$ *in F and G.*

The case represented by (2) and (3) is frequency bias induced by leakage above the Ramsey cavity. Only in this special case may the second order term *approach* the size of the linear term. Leakage either before or after the Ramsey cavity induces frequency shifts which are much larger [3, 4] and the leading order term is always linear in the microwave amplitude. To further quote from the paper by Boussert *et al*:

> Ω_r *varies linearly with the amplitude* b_p *of the perturbation and consequently with the square root of the leakage power. This result confirms that very weak leakage power may induce nontrivial shifts in clocks.*

Further in figure 11 of [3], the frequency shift is shown to be, in general, proportional to the *amplitude* of the leakage field with quadratic corrections rather than the amplitude squared term. Finally it must be noted that the results of Boussert *et al*, while highly suggestive, were originally derived for the case of a highly Doppler shifted thermal beam caesium standard and should be directly applied to a fountain style standard only with due caution. We have examined the case of leakage above the Ramsey cavity in a fountain frequency standard, both analytically and numerically, and found qualitative agreement with Boussert *et al*'s results; the frequency shift is, to first order, linear in the microwave leakage amplitude even with detunings of several tens of hertz [7].

The authors of [1] do not provide a discussion of the underlying causes of the reported frequency shift apparently depending linearly on microwave power. The paper [1] refers only to a previously observed quasi-linear frequency shift with elevated microwave power, with the measured frequency shift approaching $\delta\nu/\nu \approx 10^{-13}$ at $11\pi/2$ (with uncertainty of $\delta\nu/\nu > 3 \times 10^{-14}$) but a claimed final uncertainty of 3×10^{-6} at $\pi/2$. The authors assume a strict linearity with microwave power and make a frequency correction for microwave leakage in a primary frequency standard with magnitude of 80% of the total claimed frequency uncertainty of the standard. This correction, based only on an observed quasi-linearity of the frequency shift and without a correct underlying theory, is, in our view, highly suspect. The published data regarding the linearity of the frequency shift with microwave power are orders of magnitude too crude to justify the neglect of the term linear in the field amplitude. In the absence of any new explanation that would explain why this frequency shift should depend in a strictly linear fashion on microwave power rather than on the field amplitude, we are sceptical that the frequency shift has been correctly analysed.

In summary we firmly believe that any correction applied to a primary frequency standard must rely on a well-founded and experimentally-verified physical theory. Hence, before an observed frequency shift can be corrected, a physical, testable theory predicting that frequency shift must be advanced. Further, the fit between said theory and experiment must be excellent to the degree that the experimental data are used to correct the standard. We believe that neither of these conditions is satisfied in the reported evaluation of NPL-CSF1[1]. We note further that we are not aware of any previous report of a primary frequency standard being corrected for microwave leakage at any level.

Acknowledgments

The authors are pleased to acknowledge helpful conversations on the subject of microwave leakage with Jon Shirley, Neil Ashby, Wayne Itano, Bob Drullinger, Tom Parker, Tom Heavner, Elizabeth Donley and Tom O'Brian.

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