Measurement of the Microwave Lensing shift in NIST-F1 and NIST-F2

S R Jefferts, T P Heavner, S E Barlow and N Ashby

NIST Time and Frequency Division, National Institute for Standards and Technology, Boulder, CO 80305, USA

Steven.Jefferts@nist.gov

Abstract. With several Primary Frequency Standards (PFS) across the world demonstrating systematic fractional frequency uncertainties on order of 1 x 10^{-16} , it is crucial to accurately measure or model even small frequency shifts that could affect the ultimate PFS uncertainty, and thus ultimately impact the rate of Coordinated Universal Time (UTC) which relies on precision PFS measurements. Recently there has been controversy about the physical causes and size of PFS frequency shifts due to microwave lensing effects. We present here the first measurements of microwave lensing frequency shifts in the PFS NIST-F1 and NIST-F2. The measured frequency shifts agree well with the recent theory of Ashby et al [1].

1. Introduction

Precise determination of Coordinated Universal Time (UTC) or closely related quantities is crucial for a broad range of modern technologies such as global navigation satellite systems, telecommunications, and many other applications. The rate of UTC, and thus its precision and accuracy, is ultimately determined by about 15 Primary Frequency Standards (PFS) across the world. With several of these PFS now demonstrating systematic fractional frequency uncertainties close to 1 x 10⁻¹⁶, the ultimate accuracy of UTC and related quantities increasingly depends on the measurement and/or modelling of very small PFS frequency shifts. In recent years, the group at Penn State [2] has proposed a microwave lensing model for PFS that predicts a frequency shift in NIST-F2 of approximately $0.9 \times$ 10^{-16} , comparable to the type B fractional frequency uncertainty of 1.1×10^{-16} . A different model by Ashby et al [1] predicts a much smaller microwave lensing frequency shift, less than 0.3×10^{-16} , for both NIST-F1 and NIST-F2. The predictions of these models are sufficiently different as to potentially change the rate of UTC if applied to PFS, so it is crucial to determine as accurately as possible which model (if any) best reflects physical reality. Finally, as we note in [3], this shift is probably not amenable to calculation of a precision correction as it requires knowledge of too many unknown interaction potentials.

We describe measurements of microwave lensing frequency shifts in the PFS NIST-F1 and NIST-F2. The results of the measurement are in agreement with the prediction by Ashby et al (See figure 1). The measured lensing frequency shift is substantially smaller than the shift predicted by the model of [2]. In any case, the method used here to measure and correct the frequency bias: measuring frequency shifts at elevated odd-integer multiples of the optimum microwave levels and extrapolating to zero in order to estimate the shift at optimum microwave amplitude is a correct and robust method

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of dealing with this systematic frequency shift. Given the current state of the art of the theory of the lensing shift, the results of the measurements presented in this paper suggest that PFS frequencies should certainly not be corrected via calculation based on theory, rather any correction to the PFS frequency should rely on measured data.

2. Model and Results

Two, somewhat different, theories of the microwave lensing shift [1,2] predict frequency shifts in fountain style microwave clocks as a result of focusing and deflection of the atomic wave packets. This deflection and focusing, first predicted by Cook [4,5], results from small forces exerted on the atomic wavefunctions by the gradient of the microwave field during Ramsey excitation. Both of the two theories of microwave lensing predict a frequency shift where the frequency shift at elevated microwave amplitude shows a particular pattern. If data is taken only at a Rabi tipping angle $\phi = b\tau = n\pi/2$, with n=1,3,5,7,9 the shift scales as 1,-3,5,-7,9...etc. The frequency shift at n=3 is expected to be -3 times that at n=1. Similarly the frequency shift at n=5 is 5 times that at n=1, and the shift at n=7 is -7 times that at n=1 etc. Thus, for data taken at odd integer multiples of $\phi = \pi/2$, the pattern of frequency shifts is identical to that from microwave leakage below the Ramsey cavity [6].

Under particular circumstances microwave spurs can also mimic the predicted behaviour of the lensing frequency bias at higher microwave amplitudes [7]. As a result of these other microwave effects we have long measured our PFS frequency as a function of microwave amplitude looking for this pattern. We do this in spite of the fact that other factors preclude either microwave leakage frequency biases or spur induced frequency biases in either NIST-F1 or NIST-F2. Indeed, in both NIST-F1 and NIST-F2, microwave leakage is minimized by a large collection of techniques all of which are continuously employed so as to be sure the effect is mitigated. Schematically these fountains are quite similar and we refer to both fountains in what follows unless explicitly indicated otherwise. The minimization/elimination techniques for microwave leakage are explained in some detail in [6-9]. We review some of the major points here. In order that there be a microwave leakage frequency bias, there must, of course, be resonant microwaves present at the location of the atoms. We seek to prevent leakage induced frequency shifts using techniques that fall into two broad categories: first, don't generate any resonant microwaves and/or second, shield the atoms so that a microwave field cannot exist within the area the atoms occupy. As shown in [5] microwave leakage either before or after the two-pulse Ramsey interaction causes the pattern of frequency bias as predicted by [1,2] for measurements at odd integer multiples of optimum excitation strength. Because we state-select within the magnetic shields and finish that state-selection with an optical pulse while the atoms are in the below-cutoff waveguide between the two microwave cavities (one for stateselection and one for Ramsey interrogation, see ref [11], figure 2) we can eliminate microwave leakage before the Ramsey interaction as a source of frequency bias. Further, no field can exist within the below-cutoff waveguide except that from the Ramsey cavity. The microwave synthesizer which generates the microwaves for state-selection is attenuated and strongly detuned when the atoms are outside the state-selection area and therefore cannot induce a frequency bias. Microwave-leakage induced frequency-biases resulting from leakage above the Ramsey interaction cavity is precluded in our fountains by the design of the drift region and has a different behaviour vs. microwave amplitude in any case [5-8]. This leaves microwave leakage after the second Ramsey interaction as the only possible source of leakage induced frequency bias. This too is effectively impossible in our PFS; the microwave synthesizer that generates the Ramsey interaction microwaves is the only operational microwave source between the time the atoms enter the Ramsey cavity and the detection sequence and it is strongly detuned while the atoms are still in the below-cutoff waveguide just below the Ramsey cavity after the second Ramsey interaction (the same place the optical blast occurred on the way up). By the time the atoms exit the Ramsey-cavity below-cutoff waveguide there are therefore no resonant microwaves being generated in the experiment.



Figure 1 – Measured microwave lensing shifts (points with error bars) for NIST-F1 and NIST-F2 vs. predictions (no error bars) of various theories. The blue and black dashed lines are the results of predictions using the theory in [1] for a wavepacket size of the deBroglie wavelength (Blue) or minimum uncertainty wavepackets (Black) for the case of NIST-F1 and NIST-F2. The red dashed line is the prediction from [12]. We see good agreement between all of our data and with the theory in [1] and statistically-significant disagreement with the theory in [2,12,14]. Note that the result labelled "Measured NIST Lensing" is the weighted average of the previous 3 points labelled: NIST-F1(OLD), NIST-F2, and NIST-F1(2015). (colour online)

We have measured the spur levels and patterns in the frequency synthesizers used in both fountains [10]. None of the 4 synthesizers used in these experiments generates spurs that can cause these frequency shifts at levels of $\delta v / v > 10^{-17}$.

As a result of these considerations we can use previously measured data for NIST-F2 to estimate the lensing shift. Analysing these data for the pattern of frequency shifts predicted in [1,2] results in a measured factional frequency bias of $\frac{\delta v}{v_o} = (-0.008 \pm 0.095) \times 10^{-15}$ at n=1. Previously we have analysed these data using nonlinear weighted regression, recently we have developed a linearization technique that allows weighted linear regression to be used, and hence the change from the results reported in [10]. We take this to be a microwave lensing induced frequency bias. Ashby et al. [1], predict $\frac{\delta v}{v_o} = 0.029 \times 10^{-15}$ for this frequency bias in NIST-F2 while ref [12] predicts $\frac{\delta v}{v_o} = 0.09 \times 10^{-15}$ for NIST-F2 under similar conditions. Because these data are collected as a routine part of normal fountain operation for both NIST-F1 and NIST-F2, we have similar data for NIST-F1 as well. Treating those data in the same fashion as the NIST-F2 data, we can measure the lensing shift in NIST-F1. This results in a measured shift for NIST-F1 of $\frac{\delta v}{v_o} = (-0.019 \pm 0.083) \times 10^{-15}$ for older data (up until 2015). NIST-F1 was recently moved into a new location which resulted in a remeasurement of this bias. The re-measured point is also shown in figure 1 along with the earlier NIST-F1 and NIST-F2 have such similar microwave structures and Ramsey times, we can combine

the measured lensing shifts for the two fountains and average the Ashby results (the Ashby theory gives $\frac{\delta v}{v_o} = 0.029 \times 10^{-15}$ for NIST-F2 and $\frac{\delta v}{v_o} = 0.027 \times 10^{-15}$ for NIST-F1) giving the result shown in figure 1. Further, we have scaled the prediction for the bias in NIST-F2 found in [12] by the ratio of Ashby's F1/F2 predictions to generate our best guess as to the F1 prediction using the theory of [2,12-13]. We are forced into this unusual step, because published formulae for frequency corrections using the theory in [2,12, 14] seem to be in serious error as discussed in Appendix A of this document and in [3, 11, 13]. In [12] it is claimed that Eq. (1) (of [12]) is used to calculate the lensing frequency shift in NIST-F2. This is unlikely because Eq. (1) of [12] seems to be dimensionally incorrect, see appendix A. We fail to understand how it is possible to calculate a shift using the published expressions for the shift contained in work of [2, 12]. As shown in figure 1, while there is good agreement between the Ashby theory and our measurements, our results are not in agreement with those claimed by [2,12,14]

All existing theories of the microwave lensing bias share a common defect; they predict a frequency shift due to lensing which results from a purely mechanical "clipping" of a portion of the atomic wavepacket for a particular atom. Essentially all atoms have their wavefunctions clipped and both superposition components of the wavefunctions are clipped almost equally (if they were, in fact, equal there would be no frequency shift from clipping). Such purely mechanical clipping is, of course, only a mathematical artifice, physically any such clipping is presumably the product of an interaction between the atom and the aperture doing the clipping and the resulting interaction Hamiltonian must be evaluated. As we pointed out in [3], phase shifts from wall interactions six or more orders of magnitude greater than those required for this frequency shift have been measured. Because the wavefunction of one of the two microwave superposition states is clipped a small amount more than the other, any differential phase shift of the superposition state as a result of the clipping could easily be imposed on the superposition by the clipping. The scale and sign of the effect could therefore be vastly different from that predicted in [1,2]. The only method of dealing with this shift in a precision measurement is, in fact, to measure it. The lensing shift cannot be calculated with sufficient robustness to be confidently used in a PFS even if the theories were in agreement. In the present case where the theories disagree, this is especially true.

3. Conclusions We present the first measurements of the microwave lensing frequency shift. Three independent measurements of the microwave lensing frequency bias in two different Primary Frequency Standards; NIST-F1 and NIST-F2, are discussed. These results are reinterpretations of previously measured data along with some newly measured data in the case of NIST-F1. All of the measurements are in good agreement with the predictions made using the theory of Ashby et al. [1]. The method used to extract the lensing bias from these measurements; using the predicted behaviour of the frequency shift vs. microwave amplitude at odd integers of optimum excitation along with measurements made at those odd integer multiples of the optimum excitation is a robust and correct method for measuring the actual frequency bias from this effect. Our result, measurement of the lensing bias, is the only published experimental data on this effect at this time and it disagrees with the theory of Gibble in [2, 12, 14]. It would seem therefore that fountain corrections should not be made on the basis of calculations made using the theories of microwave lensing presented in [2,12,14] until and unless experimental evidence allows for such corrections. We would speculate that, generally speaking, frequency corrections estimated on the basis of measurements are more likely to reflect the actual reality of that particular correction in any given fountain than a (necessarily oversimplified) theoretical calculation.

Acknowledgements: We gratefully acknowledge T. Parker and T. O'Brian for many helpful comments and discussions regarding this shift. We acknowledge K. Gibble for motivating us to return to this data for reconsideration.

Appendix A We have suggested that there are multiple errors in the theory promulgated in [2, 12] as well as earlier work in [14]. Some of these errors are discussed in [3], here we discuss a few that we feel undermine the ability of the theory to be used to calculate "corrections" to PFS or SFS. This is not meant to be an exhaustive list, rather it is a limited sampling of the reasons we find the exposition of the theory lacking in sufficient rigor to be used in the calculation of corrections to PFS. Note that references to equation numbers are to the equation numbers contained in the reference under discussion.

Starting with the oldest (2006) of the references first [14], we note the following errors:

1 - First, the microwave magnetic field is defined as $B(\vec{r}) = \cos(k_{1x}x)\cos(k_{1z}z)$. The units on the two sides of the equation do not match, the left hand side (LHS) has units of magnetic field while the right hand side (RHS) has no units. Equations with different units on the RHS and LHS are, by definition, nonsense.

2 – Equations (3) and (4) are changes in probability that result from the resonant interaction of the atoms with the microwave field. However, the amplitude of the microwave field never appears in Eq. (3) or (Eq. (4), and, as a result the δP and ΔP_R as defined by the equations are *independent* of microwave field amplitude with the result that the resulting frequency shift is also independent of amplitude. This is unphysical.

3 - The entire mathematical development of theory is based on the idea that the individual atom wavepacket size is much smaller than the density distribution of atoms, this is incorrect. Consider a 1mm sized atomic cloud at launch with a 1µK temperature. Further consider that the atoms are described by minimum uncertainty wavepackets. At the end of a 0.6s ballistic flight (typical of a fountain PFS) the atomic density (cloud) size is about 0.7mm as a result of thermal spreading, while the individual wavepacket size is more than 1cm as a result of quantum mechanical spreading. Clearly, if the size of the atom-cloud density distribution matters (and the theory of [2,12,14] says it does), then so must the size of the wavepacket under the conditions that obtain in a fountain PFS. The Penn State group's theory incorrectly ignores the individual atoms in favour of the cloud density distribution. The individual atom's wavepacket sizes are never used in the calculation of the frequency shift.

Continuing with later versions of the theory (2014) we see in Ref [2], the following errors:

1 -In Eq. (4) we see the supposed frequency shift is identically zero at all times.

2 - In Eq.(6) and Eq. (7) the units on the LHS do not match those in the RHS of the equations.

Finally in the latest version of the theory (Ref [12], 2015) put forward by the Penn State group we see the following:

1 – In Eq. (2), reproduced here $\phi_1(\vec{r}) = \int_{-\infty}^{\infty} H_z(\vec{r}, z) dz$. We therefore apparently have an angle (presumably in radians) which has units of magnetic field times length on the RHS of the equation. Thus, according to [12], angle(radians)=tesla-meters or, assuming magnetic field units are in Hz (ie. Rabi frequency), then angle(radians)=velocity or some such.

$$2 - \text{In Eq (1) of [12], given as } \frac{\delta v}{v} = \frac{\phi_1}{\frac{\sin(\phi_1)}{\sin(\phi_1)}} \frac{a(t_{2L} - t_1)}{k(t_2 - t_1)}}{k(t_2 - t_1)}$$

$$\times \frac{\int_0^{2\pi} d\phi_{2L0} \int_{r_{1L} < a} \frac{r_{2L0}(t_1 - t_{1L}) + r_{1L}(t_{2L} - t_1) \cos(\phi_{2L0})}{r_1} \int_1 (kr_1) \psi_0^{-2} (\vec{r}_{2L0}, \vec{r}_{1L})|_{r_{2L0} = a} d\vec{r_{1L}} d\phi_{2L0}}{\int_{r_{2L0} < a, r_{1L} < a} \psi_0^{-2} (\vec{r}_{2L0}, \vec{r}_{1L}) d\vec{r_{1L}} d\vec{r_{2L0}}}$$

We identify a number of issues. The first term, $\frac{\phi_1}{sin(\phi_1)}$, has no units, the second term $\left(\frac{a(t_{2L}-t_1)}{k(t_2-t_1)}\right)$, has units of l^2 , The term $\frac{r_{2LO}(t_1-t_{1L})+r_{1L}(t_{2L}-t_1)\cos(\phi_{2LO})}{r_1}$, has units of time. Note this apparently must be true as $\vec{r_1}$ is defined as $\vec{r_1} = \frac{\vec{r_{2LO}}(t_1-t_{1L})+\vec{r_{1L}}(t_{2L}-t_1)}{(t_{2L}-t_{1L})}$, so that $r_{2LO}(t_1-t_{1L})$ must logically be a length times a time or $\vec{r_1}$ has units of $l \times s^{-1}$, either interpretation will leave the units in the above equation being incorrect. Returning to the equation above, the meaning of expressions like $\iint_{r_{2LO}<a, r_{1L}<a} d\vec{r_{1L}} d\vec{r_{2LO}}$ are undefined anywhere in [12] (as in fact are most of the symbols in Eq (1)). The integrals could reasonably be supposed to carry units of $l \times t, t, or t/l$ for the integrals having dimensionality of $l, l^2, or l^3$ respectively. Under any set of assumptions about the undefined notation, the fractional frequency shift should not have any units. Further errors in the same equation involve ψ_o^2 . The definition of ψ_o^2 in Ref [12] is:

$$\psi_o^2(\vec{r}_{2LO}, \vec{r}_{1L}) = e^{\frac{r_{2LO}^2 w_{1L}^2 + r_{1L}^2 w_{2L}^2 - 2r_{2LO} r_{1L} \left(w_{\Theta}^2 + u^2 t_{2L} t_{1L} \cos(\phi_{2LO})\right)}{w_o^2 u^2 (t_{2L} - t_{1L})^2}}$$

The ψ in question here is not an atomic wave function and does not describe any atom, it is, in fact, related only to the atomic cloud density distribution, and then only for an atomic cloud centred on the cavity. Further, atomic wavefunctions are generally normalized, this is not. We would contend that the use of ψ for something which is not an atomic wavefunction within the present context is a wholly unnecessary obfuscation of the theory in question. The theory in [1] deals with atoms transiting the cavity at any radial position and with transverse velocity, that is, atoms as they actually exist in fountain PFS.

Space considerations mean that we have attempted to illustrate only a subset of the errors in the theory of the lensing shift propounded by the Penn State group. These errors span the full range of time in which the Penn State group has published papers on the theory. The errors persist from the earliest paper in 2006 [14] to the most recent in 2015 [12]. We feel that in light of these errors it is impossible to use the formulae in these references to actually calculate a correction to a PFS.

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References

- [1] Ashby N, Barlow S, Heavner T and Jefferts S 2015 Frequency shifts in NIST cs primary frequency standards due to transverse rf field gradients, *Phys. Rev.* A **91** 033624.
- [2] Gibble K 2014 Ramsey spectroscopy, matter-wave interferometry, and the microwave lensing frequency shift *Phys. Rev* A **90** 015601.
- [3] Jefferts S, Heavner T, Barlow S and Ashby N 2015 Comment on 'Ramsey spectroscopy, matterwave interferometry, and the microwave lensing frequency shift' *Phys. Rev* A **91** 067601.
- [4] Cook R J 1978 Theory of Atomic Motion in a Resonant Electromagnetic Wave Phys. Rev. Lett.

41 1788.

- [5] Cook R J 1987 Optical Stern-Gerlach Effect Phys. Rev. A 35 3844.
- [6] Shirley J H, Levi F, Heavner T P, Calonico D, Dai-HyukYu and Jefferts S R 2006 Microwave leakage-induced frequency shifts in the primary frequency standards NIST-F1 and IEN-CS1 *IEEE Trans. Utrason.* 53 2376-2385.
- [7] Levi F, Shirley J H, Heavner T P, Dai-Hyuk Yu and Jefferts S R 2006 Power dependence of the frequency bias caused by spurious components in the microwave spectrum in atomic fountains *IEEE Trans. Ultrason.* 53 1584-1589.
- [8] Jefferts et al. 2002 Accuracy evaluation of NIST-F1 Metrologia 39 321-336.
- [9] Heavner et al. 2005 NIST-F1: recent improvements and accuracy evaluations *Metrologia* 42 411-422.
- [10] Heavner, T P, Jefferts, S R, Donley, E A, Parker, T E, Levi, F 2005 A New Microwave Synthesis Chain for the Primary Frequency Standard NIST-F1 Proc. 2005 Joint Mtg. IEEE Freq. Cont. Symp. PTTI 308-311.
- [11] Heavner T P, et al. 2014 First accuracy evaluation of NIST-F2 Metrologia 51 174-182.
- [12] Gibble K 2015 Comment on 'First accuracy evaluation of NIST-F2', Metrologia 52 163-166.
- [13] Jefferts S R et al. 2016 Reply to "Comment on 'First accuracy evaluation of NIST-F2'" *to be submitted to Metrologia.*
- [14] Gibble K 2006 Phys Rev Lett 97 073002.