Characterization and Reduction of Number Dependent Sensitivity in Multi-pole Linear Ion Trap Standards (LITS)

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Abstract**--The Multi-pole Linear Ion Trap Standard developed at the Jet Propulsion Laboratory has demonstrated excellent short and long-term stability and improved immunity from two of its remaining systematic effects, the second order Doppler shift and second order Zeeman shift. The technology has also demonstrated long-term operation in the field. In this paper we discuss the LITS systematic effects and present the characterization and reduction of these shifts and their dependence on ion number.**

I. INTRODUCTION

Atomic frequency standards with excellent long term stability and very low drift are needed for the generation and maintenance of timescales. The relative insensitivity to the second-order Doppler shift of Hg^+ multi-pole Linear Ion Trap Standards (LITS) developed at the Jet Propulsion Laboratory (JPL) [1] has resulted in a frequency standard with excellent long-term stability [2]. This performance has been realized even though in its present configuration the multi-pole LITS has no feedback control of the 3 largest remaining systematic effects: 1) variations in the number of ions trapped, 2) variations in the ambient magnetic field, and 3) variations in background pressure. The combined contribution of these effects to the long-term fractional frequency instability of the multi-pole LITS has been measured at $< 2x10^{-16}$/day [2]. While the multi-pole LITS frequency already has low sensitivity to the number of ions trapped, this remains the largest contributing factor to small frequency variations observed over the long term.

With initial operaton of the multi-pole LITS the number-dependent shift was characterized [3]. Though the sensitivity was low, the shift had the opposite sign expected for a second-order Doppler shift. This anomalous shift has since been demonstrated to be a number-dependent effect consisting of a combination of the ion-number-dependent second-order Doppler shift and a small contribution due to magnetic field inhomogeneity [4].

While ultimately it may be beneficial to place the ion number in a control loop, an essential first step is to reduce the sensitivity of the standard to ion-number-dependent shifts as much as possible. In this paper we present a thorough characterization of the number-dependent effect along and a demonstrated method for further reducing it.

II. MULTI-POLE LITS CONFIGURATION

The $^{199}Hg^+$ LITS is designed for continuous operation and with components that can operate for months to years without intervention. For example, the LITS uses no lasers but instead uses a $^{202}Hg^+$ plasma discharge lamp for state preparation and read-out and a helium buffer gas for ion cooling.

The multi-pole LITS has been described in detail elsewhere [1]. The physics package consists of a quadrupole trap, identical to those used in the predecessor LITS, that is used for the initial ion loading and state preparation. The ions are held near room temperature by a helium buffer gas with a partial pressure of about 10^{-5} torr. The present multi-pole trap consists of 12 rods and is an extension of the quadrupole loading trap (Fig. 1. Ions are "shuttled" between the two traps by varying their relative DC bias potentials with loading taking place in the quadrupole trap and the sensitive microwave interrogation taking place in the separate multi-pole trap. As derived in [1, 5] a key feature of the multi-pole trap is that the average rf amplitude experienced by ion cloud is smaller than in the corresponding quadrupole trap, resulting in a smaller second-order Doppler shift. Another benefit is that microwave interrogation of the ions takes place in an improved environment, well away from the contact potentials and stray light present in the quadrupole loading and state preparation trap. Microwaves to interrogate the 40.5 GHz ground state hyperfine transition are delivered to the multi-pole trap using a ceramic waveguide inside the vacuum enclosure.

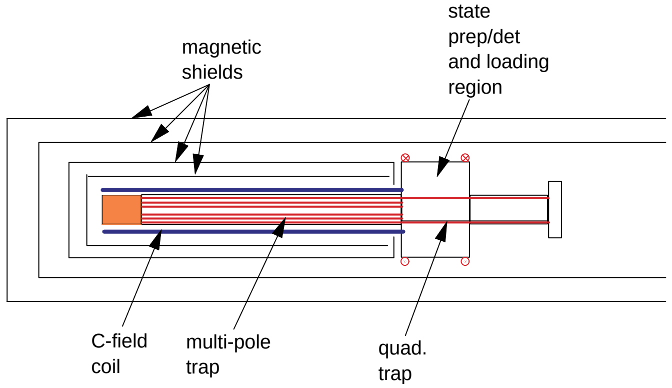

Figure 1. The multi-pole LITS physics package. Shown is a schematic of the relative positions of key components (not to scale).

Initially, two multi-pole LITS were developed at JPL, identified as LITS-8 and LITS-9. LITS-8 was delivered to the U.S. Naval Observatory (USNO) and has been operating there since 2002 [2]. LITS-9 is currently operating at the Jet Propulsion Laboratory (JPL) Frequency Standards Test Laboratory. Both LITS-8 and LITS-9 are optimized for long-term continuous operation and timekeeping applications. Smaller standards using the multi-pole trap configuration are also being developed at JPL for spaceflight applications [6-8]. A very small physics unit has recently been constructed using a sealed vacuum system showing excellent performance [9].

III. MULTI-POLE LITS CURRENT PERFORMANCE

The multi-pole LITS has demonstrated a short-term performance as low as $7\times10^{-14}/\tau^{1/2}$ and reference maser-limited long-term performance. LITS-8 operating in the clock ensemble at USNO has not deviated in fractional frequency from the USNO master clock by more than 3×10^{-14} or shown a fractional frequency drift of more than 2×10^{-16}/day [2]. While this is excellent performance, it is the intent of this paper to examine causes for residual drift with the goal of further reduction.

A. *Multi-pole LITS Systematics*

Table 1 lists known systematic shifts or limits associated with the $^{199}Hg^+$ multi-pole LITS. The stability floor for the second order Doppler shift is an upper bound since it probably includes other sensitivities (such as to He pressure stability). The He pressure shift is the next largest systematic effect. While not discussed in detail here, LITS-9 is being converted to use neon for its buffer gas. The neon pressure shift is approximately 3x smaller than the helium pressure shift [11] and because of its mass, it cools the mercury ions more efficiently enabling operation at a lower buffer gas pressure. Neon will be introduced via a capillary leak instead of the heated quartz leak currently used for helium, which should further improve stability.

TABLE I. Systematic fractional frequency shifts for the $S_{1/2}$ F=0,mF=0 - $S_{1/2}$ F=1,mF=0 microwave clock transition in the multi-pole Hg^+ LITS. The He pressure shift assumes a background partial pressure of 10^{-5} torr of He. Pressure shifts for other gas species assume partial pressures of less than 10^{-9} torr. The light shift estimate assumes a lamp output (dim state) of 100 µW/cm^2 with a 1 GHz spectral width 3 GHz detuned from the 194 nm 6s $^2S_{1/2}$ – 6p $^2P_{1/2}$ optical transition and an ion temperature of 500 K. The estimate also assumes that light reflected from the loading region into the sensitive interrogation region is attenuated by more than 10^4. A C-field of 80 mG is used for Zeeman calculations. The rf AC Zeeman and Stark shifts assume a 1 MHz rf amplitude of 35 V.

Shift	Scaling	Magnitude	Systematic Floor
Second order Doppler shift – mulit-pole trap [5]	$-\langle v^2/c^2\rangle$	-1×10^{-13}	$<5\times10^{-16}$
He pressure shift [10, 11]	P_{He}	3×10^{-13}	$<2\times10^{-16}$
Hg Pressure shift	P_{Hg}	?	$<2\times10^{-16}$
Other pressure shifts (H, N, CO, CO_2, CH_4, etc.) [11]	P_{other}	$<10^{-16}$	$<10^{-16}$
194 nm light shift (est.)	I_{194}	2×10^{-16}	2×10^{-17}
Second order Zeeman shift [4]	$\langle B^2\rangle$	1.5×10^{-11}	1.5×10^{-17}
Black Body Shift [12]	$-T^4_{ambient}$	-1×10^{-16}	1.3×10^{-19}
rf AC Zeeman shift	$\langle B^2_{rf}\rangle$	$<2\times10^{-13}$	$<2\times10^{-19}$
rf AC Stark shift [12]	$\langle E^2_{rf}\rangle$	$<10^{-19}$	$<10^{-19}$

IV. ION-NUMBER-DEPENDENT EFFECTS

Previously, the second order Doppler shift effect was characterized in the LITS by varying the ion number. However there are three ways that varying the ion number can affect the LITS clock frequency. The second order Doppler shift in an ion trap has two components: one due to the temperature of the ions, which is indirectly related to the ion number, and the other due to geometric effects that are exacerbated by trapped ion number changes. For the second component, as ion number is increased, space charge repulsion causes the ion cloud volume to increase, thereby increasing the average rf trap amplitude seen by the ions. The amplitude of the ion micro-motion is proportional to the rf trap potential, hence a number-dependent second order

Doppler shift. Since this effect scales with $-\langle v^2/c^2 \rangle$ a second order Doppler shift has a negative slope when plotted against ion number. This effect is greatly reduced in a multi-pole trap because the trap potential approximates a square well and the average rf amplitude seen by the ions is much smaller than in a quadrupole trap.

A third ion number effect is magnetic. Great care is taken in the multi-pole LITS to create a uniform C-field with a solenoid. Unfortunately, due to the finite solenoid length some fringing in the field exists at the ends, which overlap the trap. As the ion number is increased, the ion cloud volume increases and now experiences a different value of $\langle B^2 \rangle$ where the average is taken over the ion cloud volume. Fig. 2 shows this effect schematically.

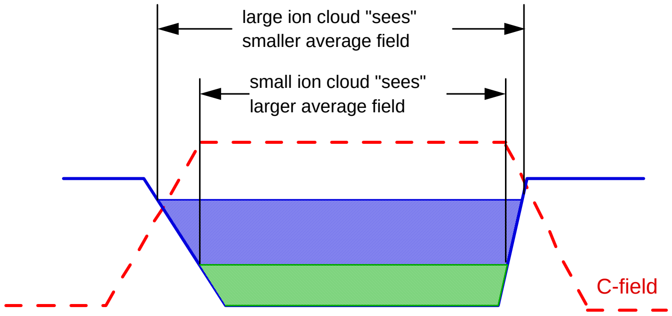

Figure 2. A cross section of the trap potential in the axial direction superimposed with a C-field that has fringing at the ends. As the ion cloud volume increases the value of $\langle B^2 \rangle$ decreases and so does the second order Zeeman shift. The effect is conceptually similar, though smaller, in the radial direction.

Due to fringing, $\langle B^2 \rangle$ decreases with ion cloud volume and therefore with ion number as well, leading to a decreasing second order Zeeman shift. In this case the slope of the shift when plotted against ion number is negative as with the number-dependent second order Doppler shift. However the ends of the solenoid are also very close to the endcaps of the inner two magnetic shield layers, which can cause a slight field increase. If the field increases near the solenoid ends then the slope of the magnetic inhomogeneity effect will be positive. Thus, the combination of the number-dependent second order Doppler shift and the number-dependent second order Zeeman shift can lead to either a positive or negative slope. The number-dependent effect in the multi-pole LITS has been correlated with changes in the average magnetic field using the field-sensitive m=0-m=±1 transitions [4].

A. Ion-number dependence in LITS-8

The method used most often to vary the number of trapped ions is to change the trapping potentials, typically the endcap DC bias voltage for the load trap. While this does vary the ion number, it also impacts other ion cloud characteristics such as temperature. To rule out the possibility of another systematic effect "masquerading" as an ion-number-dependent effect, it is useful to have an orthogonal way of varying ion number. One approach is to vary the temperature of the mercury oven, however the time required to reach equilibrium is long and this approach was generally not used. However, recently the mercury source was replenished in LITS-8 at USNO. The mercury oven temperature was subsequently increased in several steps over a six-month period. During this time, the LITS-8 frequency offset was monitored allowing this orthogonal measurement of ion-number dependence. Fig. 3 shows the clock resonance signal size and frequency offset plotted on the same graph.

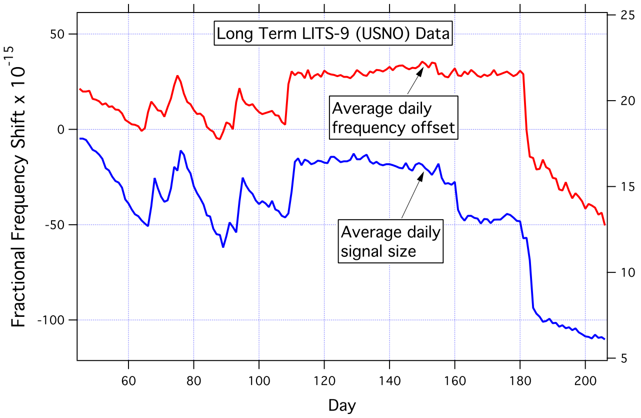

Figure 3. Fractional frequency shift and signal size data for LITS-8 over a six-month period from November 2004 to May 2005. Frequency offsets are measured from an H-maser referenced to the USNO master clock. Signal size is assumed to be proportional to trapped ion number. Jumps in the signal size before day 120 were due to discrete changes in the mercury oven temperature. The signal size change at day 180 was due to an electronic problem which reduced the trapping potential.

The total frequency shift from an empty to full trap is about 3 mHz or a fractional frequency shift of about 7.5×10^{-14}, which is the same as found by varying the load trap potential. The correlation between the frequency offset and changes in signal size (due to discrete changes in the mercury oven temperature), which is assumed proportional to ion number, is evident. This implies that most of the frequency deviation from the USNO master clock observed previously is due to this effect. In-as-far as we are able to mitigate ion-number dependence, we are likely to improve stability by equal measure.

One notable event where the correlation does not hold occurs at day 160. Here the signal size makes a discrete jump while the frequency remains stable. Clock telemetry for this time period shows that the total light level (signal size plus background) changed by more than the drop in signal size alone indicating a change in the lamp output. Changes in lamp state are not uncommon and the frequency algorithm is immune to lamp output variations to second order. We conclude that the lack of correlation at this one point is due to a lamp state change and not an ion number change.

V. MODELING ION NUMBER DEPENDENCE

Having verified that the long term frequency stability is affected by changes in ion number and that the sensitivity has a magnetic component, we turn to modeling the effect of magnetic field inhomogeniety in the multipole region of the physics package. The trap, solenoid, and shields have azimuthal symmetry allowing use of a 2-D finite element model to determine the field everywhere in the volume contained by the quadrupole and multi-pole traps. The model includes the magnetic shields, the C-field solenoid and a number of auxiliary coils that will be described below. These represent the components that determine the magnetic environment of the physics package except external perturbations, which are small on the scale of interest.

Since we expect the magnetic effect to be determined by field inhomogeneity at the ends of the C-field solenoid and inner shields, we add into the model an auxiliary coil at each end of the multipole trap interrogation region to modify the field at these locations. We refer to the coil at the interface between the quadrupole and multi-pole traps as AUX1 and that at the other end as AUX2. Fig. 4 shows the magnitude of the modeled field along the axis of the physics package.

The region from z = 0 m to z = 0.38 m corresponds to the multi-pole trap region where the microwave interrogation takes place. This figure shows how the field is quite uniform at the lower end (z = 0), but not as uniform at the upper end. While improved uniformity will be designed in the next standard, the addition of a trim coil can significantly reduce non-uniformities. The dashed line shows improved uniformity with the application of a current in AUX1.

The average frequency shift for the second order Zeeman shift in Hg^+ is:

$$\langle \Delta f \rangle = 9.7 \times 10^9 \frac{Hz}{T^2} \langle B_0^2 \rangle, \qquad (1)$$

where the average of the field squared is taken over the volume of the trap occupied by the ions. Fig. 5 shows how this average frequency shift varies with axial occupation. Each curve represents one setting on the AUX1 coil.

Fig. 6 shows the same information, but now keeping the axial occupation fixed at about 95% of the trap length and instead varying the radial occupation.

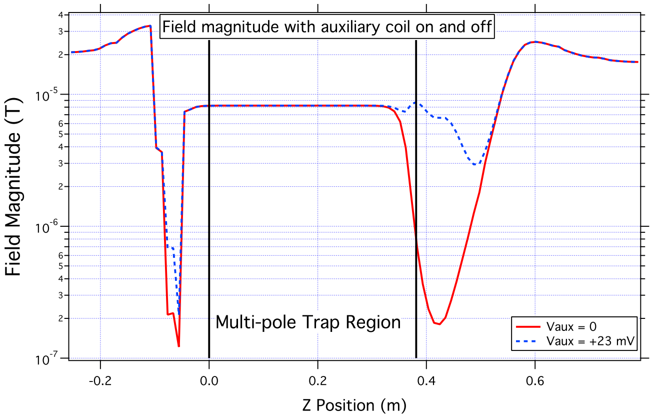

Figure 4. A plot of the modeled magnetic field magnitude along the axis of the LITS-9 physics package. The solid red line shows the field with only the C-field on. The dashed blue line shows that field modified by the application of the auxiliary coil at the interface between the quadrupole and multi-pole traps, which is also at one end of the C-field solenoid (AUX1). The axial position of 0 m corresponds to the lower end of the C-field solenoid (left side as viewed in the figure) and the region between the vertical black lines corresponds to the multi-pole trap.

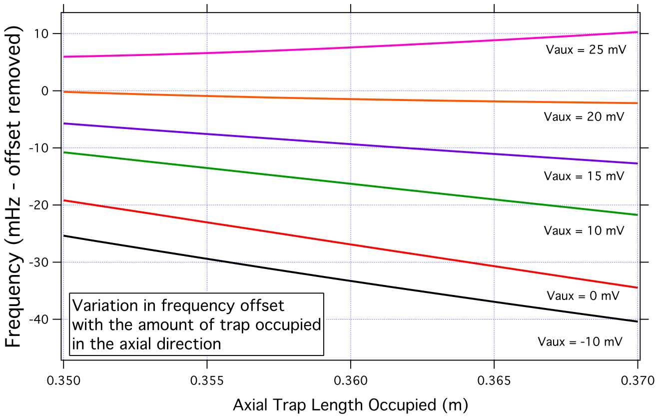

Figure 5. The average frequency shift modeled for various values of AUX1 current. Each curve plots the average frequency shift as a function of axial occupation (symmetric about the axial center point of the trap) for a single value of current in AUX1. In each case the shift is relative to a 40.5 GHz transition frequency. A frequency offset has been removed from each curve.

As the ion number is changed, space charge repulsion will cause the ion cloud to change its occupation volume in the trap. Each curve in Fig. 5 and 6 can be viewed as qualitatively showing how frequency will vary with ion number for a particular setting of the AUX1 coil. The axial data (Fig. 5) focuses on a small region near the end of the trap. The model implies that for both directions of ion cloud expansion we should be able to use AUX1 to change not only the magnitude of the number-dependent shift, but its slope as well. This suggests that in addition to simply improving field homogeniety, we may also reduce the component of the number-dependent second order Doppler shift that depends on trap geometry. The compensated system should yield a very small total ion number-dependent effect.

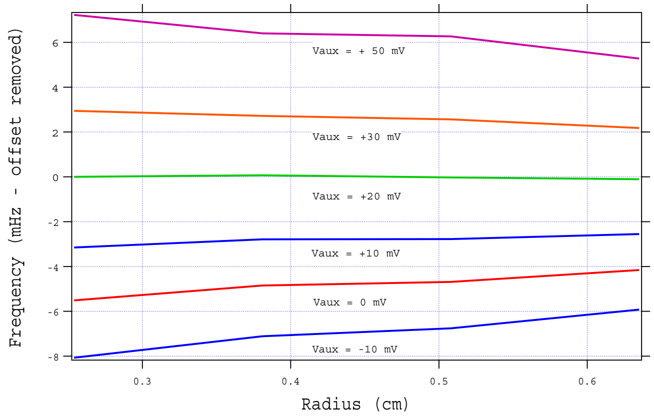

Figure 6. The average frequency shift modeled for various values of AUX1 current where each curve now represents a fixed axial occupation and a varying radial occupation. As before the shift is relative to a 40.5 GHz transition frequency. An offset between each curve as well as an overall offset has been removed so as to better show the relative changes in slope.

VI. MODIFYING THE MAGNETIC FIELD ENVIRONMENT

To test these predictions a coil was recently installed on LITS-9 at the AUX1 location. Data was taken before degaussing the magnetic shields (Fig. 7) and after (Fig. 8).

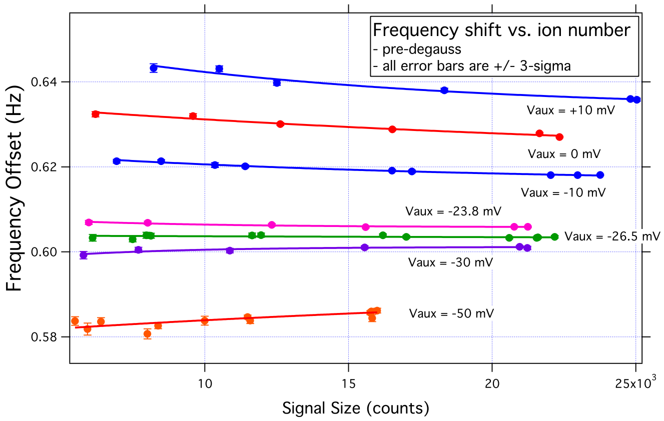

Figure 7. Measured LITS-9 frequency shifts as a function of ion number (signal size) for various AUX1 coil settings (each curve corresponds to one value of the current in AUX1) before degaussing the magnetic shields. All shifts are relative to the 40.5 GHz Hg^+ clock transition frequency. The data shows good agreement with the modeled radial data (Fig. 6).

The data show good agreement with the model that assumes the cloud expands in the radial direction, but more importantly demonstrates control over the ion-number frequency shift. The fact that the data remains qualitatively the same before and after shield degaussing indicates that the nature of the field non-uniformity is not being affected by the degaussing process. As predicted by the model, the AUX1 coil allows control not only of the offset, but also the slope of the frequency shift vs. ion number curve thereby making it possible to cancel the two effects and greatly reduce the ion-number dependence.

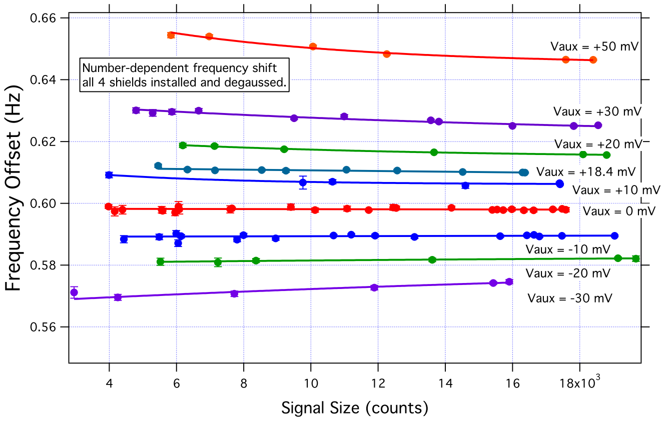

Figure 8. Measured LITS-9 frequency shifts after the magnetic shields have been degaussed. All shifts are relative to the 40.5 GHz Hg^+ clock transition frequency.The picture remains qualitatively the same, but a different overall offset is introduced.

A. *Optimal coil setting for minimal number-dependence*

Fig. 9 shows data taken at the optimal AUX1 coil setting (producing best cancellation of number-dependence). The absolute setting depends on several factors, including magnetic environment, degaussing history, and trap, C-field, and shield geometry and must re-determined for each situation. The overall shift in this data is 0.2 mHz, or a fractional shift of $5x10^{-15}$, but within the measurement uncertainty the data is consistent with no shift at all. Even a total 0.2 mHz shift represents an order of magnitude improvement over behavior with the AUX1 coil off.

It is essential to point out that cancellation schemes are only as good as they are stable. In this case, long-term data must be taken to verify that the optimal AUX1 coil setting doesn't vary with time. The largest potential contribution to variation would be a change in the magnetic environment. While this might be a concern for a portable standard, the magnetic environment in a laboratory and specifically that of the Frequency and Timing Test Laboratory at JPL, is quite stable. We anticipate that after degaussing the magnetic shields the coil setting should not need to be changed. Long-term measurements will be made to demonstrate this. Initial measurements show a relative agreement between LITS-9, UTC(NIST) and UTC(USNO) as measured using GPS time transfer to be better than $2x10^{-16}$/day over a 20 day period.

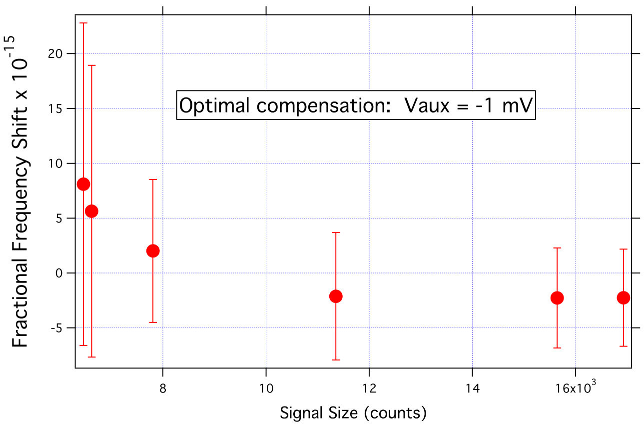

Figure 9. Frequency shift vs. ion number (signal size) data for the optimal AUX1 coil setting (minimal ion-number dependence). Each data point represents 6 hours of data with the error bars representing 3-σ statistical errors.

VII. ESTIMATING THE NUMBER-DEPENDENT SECOND-ORDER DOPPLER SHIFT IN THE 12-POLE TRAP

In addition to estimating optimum cancellation the model can also indicate the coil setting that gives the best field uniformity. Measuring the ion-number dependent shift at this setting provides and unmasked estimate of the actual ion-number-dependent second order Doppler shift alone with no magnetic contribution. Fig. 10 shows the second order Doppler shift using data taken in this way.

As expected the data shows the dramatic improvement in this effect between the quadrupole LITS and the multi-pole LITS [1]. The "compensated" multi-pole data shows the potential improvement in stability that might be obtained using AUX1 compared to current multi-pole LITS performance [2]. For instance, if the ion number is stable to 1%, then the fractional ion-number-dependent shift in the current multi-pole LITS would be 3x10^{-16}, whereas the same effect in the compensated trap would be <5x10^{-17} (measurement limited by statistical error).

VIII. CONCLUSIONS

In this paper we have verified that the source of the "anomalous" second order Doppler shift is in fact magnetic inhomogeneity. Using a finite element model we were able to pinpoint the source of the inhomogeneity and suggest an auxiliary coil configuration that would reduce it. Implementing this coil allowed an estimate of the non-magnetic number-dependent second order Doppler shift and shows that it is approximately 100x smaller in the multi-pole LITS than in the quadrupole LITS. Further, this coil allowed a means to compensate this shift reducing ion-number dependence in the multi-pole LITS by an additional order of magnitude. Work is underway to measure the long-term stability of this LITS against UTC(USNO) and UTC(NIST).

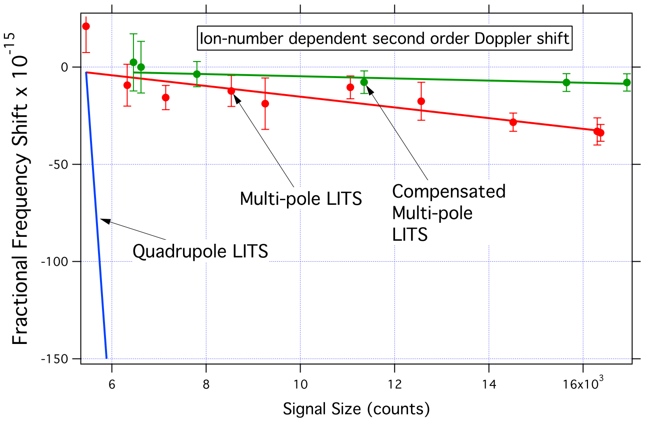

Figure 10. The ion-number-dependent second order Doppler shift for the quadrupole LITS (blue), the multi-pole LITS operating with AUX1 set to produce the most uniform field (red) and the multi-pole LITS operating with AUX1 set to produce optimal cancellation of the number-dependent effect (green). The total fractional frequency shift is about 3x10^{-12} for the quadrupole LITS, 3x10^{-14} for the multi-pole LITS and 5x10^{-15} for the "compensated" multi-pole LITS.

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