Systematic Effects in Atomic Fountain Clocks

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Abstract. We describe recent advances in the accuracies of atomic fountain clocks. New rigorous treatments of the previously large systematic uncertainties, distributed cavity phase, microwave lensing, and background gas collisions, enabled these advances. We also discuss background gas collisions of optical lattice and ion clocks and derive the smooth transition of the microwave lensing frequency shift to photon recoil shifts for large atomic wave packets.

1. Introduction

Cesium fountain clocks currently establish the frequency accuracy of International Atomic Time, TAI. The accuracy of fountains has improved by about a factor of two in the last five years. It is noteworthy that the recent accuracy improvements are largely due to new treatments that can rigorously evaluate previously significant systematic errors. Most prominent are frequency shifts due to distributed cavity phase [1-5], microwave lensing [4-8], and background gas collisions [9-14]. We review each of these and describe approaches to evaluate these frequency shifts. Regarding microwave lensing, here we explicitly show the connection of the microwave lensing frequency shift to photon recoil shifts, addressing some recent controversy about the evaluation of this frequency shift [8,15-19]. Our treatment of background gas collision shifts applies to optical lattice clocks, and may be useful for ion clocks and other precision measurements. We discuss these and close with a summary of several implementable design considerations for fountains that facilitate accuracy evaluations.

2. Frequency Shifts due to Distributed Cavity Phase

Distributed cavity phase (DCP) shifts are a first order Doppler shift due to small travelling waves in the microwave clock cavity and the motion of the cold atoms. Known for 40 years, measurements and calculations only recently agreed [1-5]. To accurately calculate the microwave fields, we first express the field as a superposition \( H(r) = H_0(r) + (\Delta \omega / T + i) g(r) \) of a pure standing wave \( H_0(r) \), for no cavity losses, and a field due to the feeds and wall losses \( g(r) \) [1,2]. Because the losses are small, it is important to separately solve finite element models of \( H_0(r) \) and \( g(r) \). Second, \( g(r) \) is decomposed into an azimuthal Fourier series \( g_z(r) = \sum_m g_{m,0}(r,z) \cos(m \phi) \) [1,2]. Because the atoms are restricted to the center of the cavity and \( g_{m,0}(r,z) \) is proportional to \( r^m \) for small \( r \), only \( m = 0, 1, \) and \( 2 \) DCP shifts are significant. Three densely-meshed 2D finite-element solutions for \( g_{m,0}(r,z) \) thus provide the full 3D solution and require dramatically fewer resources than a direct 3D solution [1,2].

The symmetry of each azimuthal Fourier component corresponds to particular effects in the fountains that produce DCP shifts. The transverse \( m=0 \) phase variations are negligible, but the longitudinal phase gradients are large and, in combination with the transverse variation of the Rabi pulse area, lead to large shifts in most clocks near \( (4,8,12) \pi / 2 \) pulses. These shifts cannot be reduced with more azimuthally distributed feeds – more longitudinally distributed feeds are required [2,20].
Since the symmetry of the m=0 phase gradients suppresses DCP shifts for π/2 pulses, the small m=0 DCP uncertainty often comes from potential top-bottom resistance inhomogeneities in the cavities [4,5,7], which can be most sensitively probed near (2,6)π/2 pulses. The m=1 variations are phase gradients, which combine with fountain tilts to produce DCP shifts that are naturally large [2-5]. The m=1 gradients from the feeds usually have a large dependence on microwave amplitude and it is helpful to use this to vertically align the fountain, along a single axis with two independent feeds [3,4,17] and along two horizontal axes with four independent feeds [2,20,21]. To exclude m=1 phase gradients from resistance inhomogeneities, the tilt sensitivity of the fountain is measured for π/2 pulses and nulled by adjusting the relative feed amplitudes [2,3]. Measurements at a higher amplitude (5π/2) do not generally exclude large m=1 shifts for π/2 pulses. Quadrupole m=2 phase variations produce DCP shifts primarily via detection inhomogeneities and offsets of the initial cloud position and are generally small enough that they can be accurately calculated [3-5,7]. Aligning the cavity feeds at 45° relative to the detection laser beams usually gives negligible m=2 DCP errors.

Stringent verification of our complete model led to significantly smaller systematic errors [3-5] and gave confidence to construct improved cavity designs with much smaller longitudinal phase gradients [2,20,21]. The most important feature to add is feeding clock cavities with 4 or more independent cables so that the fountain can be precisely aligned to be vertical along two horizontal axes. Several of the latest fountains have used the new cavities, and are consequently realizing more precise vertical alignments and observing much smaller microwave-amplitude-dependent frequency shifts [21].

3. Microwave Lensing Frequency Shifts
The microwave photon recoil shift of δω/ω=1.5×10^{-16} is now comparable to fountain clock inaccuracies and most accurate fountains contributing to TAI correct for this frequency bias. Because atoms in a fountain are localized to less than a microwave wavelength, the resonant microwave dipole forces do not yield resolved photon recoils, but instead act as weak focusing and defocusing lenses on the atom wave packets. The resulting shift depends on the clock geometry and is typically 6×10^{-17} to 9×10^{-17} for fountains [4-8,17], and larger for the microgravity clock PHARAO, 11.4×10^{-17} [22].

There is currently some controversy since the recent NIST treatment [16,18] predicts a much smaller shift, 1.6×10^{-17}, disagreeing with the prior results [4-7,17]. The NIST treatment and two recent fountain accuracy evaluations have considered that the microwave lensing shift goes to zero in the limit of zero microwave amplitude [12,15,16,19]. In [8] we explicitly derived that, while the microwave lensing of wave packets goes to zero in the limit of zero microwave amplitude, the frequency shift is non-zero because the perturbation of the transition probability δP is proportional to the lensing and the frequency shift is δP divided by the Ramsey fringe amplitude, which also goes to zero. Here, we give a simplified derivation of the microwave lensing frequency shift that is specific to weak fields. This is a fundamental limit and demonstrates the smooth connection of microwave lensing shifts to well-known photon-recoil shifts as atomic wave packets become large. Since recoil shifts are non-zero for weak fields, this connection supports the microwave lensing shift being non-zero in this limit and serves as a valuable check of numerical factors and the sign of calculated microwave lensing shifts.

We consider a small atom cloud on the fountain axis and 1D standing waves cos(kx), with general wave vectors in the first(second) Ramsey interactions. Following [6,8], but using the bare atom basis |g⟩ and |e⟩, small Ramsey pulse areas φg and φe imply that we need to only treat opposing single photon-recoils ±k_{g,e}, cos(k_{g,e}x)=½exp(ik_{g,e}x)+½exp(−ik_{g,e}x), which destructively interfere for small x to produce the lensing shift [6]. In momentum space, the detected excited-state wave function, just after the second Ramsey pulse φg, is ψ_g(k,t_z=t_1+T)=−(i/2)exp[i(kx−hk^2t_2/2m−χ/2)] [φ_g exp(−iω_eT+iχ) cos(kx−kv_N T) + φ_e cos(kx)], using the microwave photon-recoil velocity v_N=hc/√2, the photon recoil shift ω_e=hc/√2, and χ as the phase shift of the second Ramsey pulse [8]. Constructing a wave packet by integrating over k with a weight exp(−k^2/2σ_w^2) gives ψ_g(k,t_z)=A exp(−x^2/2σ_w^2) [φ_g exp(−iω_eT/τ_1+iχ) cos(kx/τ_1) + φ_e cos(kx)], where the complex wave
packet sizes are $\bar{w}_{1,2} = \hbar t_{1,2}/m\sigma + \sigma$, at the two Ramsey interactions. The excited state probability $|\psi_x(k,t)\rangle$ yields a Ramsey fringe with a frequency shift:

$$\delta \omega = \frac{1}{T} \phi \phi \int_0^T \cos(k_{n,x}) \sum_{z} \frac{x^z w_{1/2}^z}{w_2^z} \sin \left( \frac{k_x x \pm \omega_0 T}{w_2^z} \right) dx$$

Here, $w_2 = |\bar{w}_2|, w_{1/2}^z = \hbar^2 t_{1/2} / m^2 \sigma_z^2 + \sigma^2$, and $2a$ is the width of the detection aperture. The numerator is the perturbation of the transition probability due to lensing and the denominator is the Ramsey fringe amplitude. Both go to zero as $\phi \phi \phi \phi$, yielding a non-zero frequency shift in the limit of zero microwave amplitude [6,8,17], in contrast to [12,15,16]. Additionally, the NIST treatment gives zero frequency shift for all $V_x$ and $a/w_2$ in Fig. 1 since the atoms are centered on the cavity axis and [18] neglects the variation of the dipole force over the wave packets [19]. Fig. 1 shows that detecting only the center of a wave packet $(a/w_2, w_{1/2}, w_2)$ yields a microwave lensing frequency shift of $\omega_{lt}/T$ [6,8]. As $\sigma$ grows, the spread $w_2$ decreases, yielding minimal clipping of atoms and no frequency shift [6]. If $\sigma$ would grow beyond a very large 5mm, the aperture would again clip the atom wave packets and the frequency shift goes to the value of the recoil shift $\omega_h$.

4. Frequency Shifts due to Background Gas Collisions

Precision measurements with cold atoms, including fountains, optical lattice, and quantum-logic ion clocks, have a different sensitivity to background gas collisions than room-temperature clocks because background gas collisions prevent cold atoms from being detected. Therefore, room-temperature background gas collision shifts [23] do not apply to cold-atom clocks. We have derived analytic
expressions for background gas collision shifts of cold atoms and have shown that there is a highly useful proportionality between background gas shifts and atom loss rates [9]. The shifts are essentially independent of the background gas, except potentially for helium. Lifetime measurements can therefore set accurate uncertainties due to background gas frequency shifts [10-14].

The potential momentum transferred to laser-cooled atoms in fountains and lattice clocks from a background gas collision is large. In fountains, atoms that acquire velocities greater 3 cm/s are not detected and for lattice clocks, ~10 cm/s. These velocities are sufficiently low that the scattering is quantum mechanical and a partial wave expansion is useful. The quantum scattering can be separated into two contributions – the usual scattered current \( j_{sc} \) and the interference between the scattered amplitude and the unscattered amplitude in the forward direction [9]. The interference current \( j_{int} \) describes the loss of atoms due to background gas scattering, and for clocks, importantly includes a phase shift of the clock coherences. For fountains and lattice clocks, the detected scattered current is negligible and only the interference current is significant. The interference current gives a frequency shift proportional to \( \sin(2\delta_{e})-\sin(2\delta_{g}) \), which is approximately \( 2(\delta_{e}-\delta_{g})\cos(2\delta_{e}) \) for small \( \delta_{e}-\delta_{g} \), where \( \delta_{e} \) and \( \delta_{g} \) are the \( \ell^{th} \) partial wave phase shift. For small angular momenta \( \ell \), corresponding to hard short-range collisions, the phase shifts become large and the frequency shift averages to zero. Only weak long-range collisions with \( \delta_{e},\delta_{g}\leq1 \) contribute to the collision shift. The short-range collisions give large momentum transfers and have cross sections proportional to \( \sin^{2}(2\delta_{e}) \), which averages to \( \frac{1}{2} \), not 0. Including both, we get a relationship between the frequency shift and the loss of cold atoms [9]:

\[
\langle j_{int} \rangle = -0.38n \left( \frac{\mu k_{B} T}{h^2 m_p^3} \right)^{\frac{1}{2}} \left[ 3 \left( C_{e}^{g}\frac{C_{g}^{e}}{C_{e}^{g}} \right) \sin(2\delta_{g}) + 13.8 \left( C_{e}^{g} + C_{g}^{e} \right) \cos^{2} \left( \frac{Z}{2} \right) \right].
\]

Here, \(-C_{e,g}/R^6\) is the van der Waals interaction of the clock states with the background gas atom of mass \( m_p \), and \( \mu \) is the reduced mass. In room temperature clocks, the entire scattered current is detected and, combined with \( j_{int} \), gives a frequency shift proportional to \( \sin(2\delta_{e}-2\delta_{g}) \), which does not average to zero for \( \delta_{e},\delta_{g}\geq1 \) if \( \delta_{e}-\delta_{g} \) is small [9]. For microwave clocks, both clock states have the same electronic structure and \( (C_{e}-C_{g})/C_{e} \) can be bounded by \( h\omega(E_{1}-E_{0})^{-1}(E_{1}+E_{0})^{-1} \), where \( E_{1} \) and \( E_{0} \) are the lowest resonant excitations of the clock and perturber [9]. For microwave clocks, this leads to a simple expression of \(-\delta_{e}-\delta_{g}=2\times10^{-16}\Delta A\), where \( \Delta A \) is the loss of Ramsey fringe amplitude during the Ramsey interrogation time [9].

While ion clocks trap atoms sufficiently strongly to retain atoms that have hard collisions with background gas atoms or molecules, quantum-logic detection [24] can exclude ions that change their trap state. This gives a tremendous immunity to background gas shifts, because the scattering phase shifts are given by strong long range \(-C_{e,g}/R^6\) interactions, which are identical for both clocks states. The frequency shift is again given by \( C_{e-g}/C_{e} \), which gives very small \( \delta_{e}-\delta_{g} \) for \( \delta_{e},\delta_{g}\leq1 \) [9].

5. Conclusions

The many collective experiences described above have lead to a number of ways to facilitate accuracy evaluations of fountains. Many are easy to implement, especially during the design stage. Explicitly designing a method to insure that the atom cloud travels vertically through the fountain can improve and reduce the time required for accuracy evaluations. The best current recommendation is to use at least 4 independent cables to have opposing cavity feeds along both horizontal tilt axes [2, 21]. Orienting four cavity feeds to be at 45° to the orthogonal detection laser beams and fluorescence collection minimizes \( m=2 \) DCP shifts, likely to a negligible level. Together, these allow measurements of \( m=1 \) DCP shifts and negligible \( m=2 \) shifts so that only the small \( m=0 \) shifts need to be calculated, combined with limits on top-bottom resistance inhomogeneities, which are measured near (2,6) \( \pi/2 \) pulses. We note that finite-element calculations are much less intensive for cylindrically symmetric cavities, and further helped if they have no sharp corners and exclude atom trajectories that experience large microwave fields near cavity walls [1,2]. The improved and recently-implemented cavity designs [20,21] reduce the longitudinal phase gradients, and even allow for some adjustment. Such a cavity
could enable a convincing measurement of the microwave lensing frequency shift at elevated microwave amplitudes, such as $5\pi/2$ pulses, especially when combined with two state preparation cavities that can vary the atomic density and prepare the atoms in either the F=3 or 4 mF=0 state [6,8].

Several recommendations are related to the vacuum chamber. Elegant methods [25,26] have been used to evaluate the cold-collision frequency shift [27]. Using a small MOT, which could be loaded from a slow beam, has produced small uncertainties [12,21] and avoids slow drifts of the atomic distribution, which produces an unstable effective fountain-tilt and potential m=1 DCP shift [3,7]. A 111 launch [27] has some advantages; opposing laser beams can be aligned irrespective of the other beams and generating the beams is marginally simpler. Constructing the vacuum chamber with two ion pumps, with associated valves, helps to assess the background gas collision shift [10]. To reduce microwave leakage shifts, it is advantageous to control the electromagnetic mode structure in the fountain, from the clearing pulse, through the interrogation time, to the state detection. A series of cutoff waveguides, possibly including detuned microwave cavities [28], can be used. More precise measurements of blackbody coefficients and temperature measurements, as in recent lattice clocks [14,29], may be useful in the future. Finally, juggling atoms [30] significantly improves the short-term stability [31], but this technique requires more effort than the methods above.

In summary, fountain accuracies have advanced significantly over the last few years by rigorously evaluating the systematic errors due to distributed cavity phase, microwave lensing, and background gas collisions. The m=0 and 2 DCP shifts can be calculated and frequency measurements with tilted fountains at optimal amplitude set the m=1 uncertainties. We also have calculated microwave lensing frequency shifts and here we have shown a direct connection to photon-recoil shifts for large wave packets. This connection gives valuable confidence to the corrections that are applied to the majority of the accurate fountain standards contributing to TAI. The treatment of background gas collisions for fountains is also applicable to lattice clocks [13,14], and potentially to quantum-logic ion clocks [24].

Looking forward, the anticipated future redefinition of the SI second on an optical or higher frequency transition is an important motivation to continue to operate and improve cesium standards. At present, a number of systematic are becoming more difficult, especially considering the averaging times required by many fountains to reach their reported accuracies, and therefore the rate of future improvements is not clear. One could reasonably argue that fountains will not improve dramatically beyond the current $10^{-16}$ level. However, if a redefinition is still years away [32], the current limits are not fundamental and history suggests that fountain accuracies will continue to improve significantly.

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