Power Dependence of the Frequency Bias Caused by Spurious Components in the Microwave Spectrum in Atomic Fountains

Filippo Levi, Jon H. Shirley, Thomas P. Heavner, Dai-Hyuk Yu, and Steven R. Jefferts, *Member, IEEE*

***Abstract*—The presence of spurious spectral components in the microwave excitation may induce frequency shifts in an atomic fountain frequency standard. We discuss how such shifts behave as a function of power variations of the excitation carrier and in the spur-to-carrier ratio. The discussion here is limited to the case of single-sideband spurs, which are generally much more troublesome due to their ability to cause frequency shifts. We find an extremely rich and unintuitive behavior of these frequency shifts. We also discuss how pulsed operation, typical of today's fountain frequency standards, relates to frequency shifts caused by spurs in the microwave spectrum. The conclusion of these investigations is that it is, at best, difficult to use elevated power microwaves in fountain frequency standards to test for the presence of spurs in the microwave spectrum.**

I. Introduction

For the past several decades, primary frequency standards have been based on thermal atomic cesium beams. Operating these standards at high microwave power (at Rabi pulse areas well above $\pi/2$) to enhance the evaluation of potential frequency biases was unrealistic because of the large spread in atom-microwave interaction times. (This is due to the wide thermal velocity distribution in these standards.)

With the advent of atomic fountain primary frequency standards, it has become possible to operate at greatly elevated microwave power levels (pulse areas up to $13\pi/2$ are common), thanks to the extremely narrow velocity distribution attainable with laser cooling techniques. In a typical Cs fountain primary frequency standard, a sample of cold atoms passes through the Ramsey cavity at a speed of $\sim$3 m/s with spread in velocity due to the thermal distribution of only $\sim$1 cm/s.

Experiments where the Rabi frequency of the atoms in the microwave field is varied to many times the optimum (with pulse areas ranging from $\pi/2, 3\pi/2, 5\pi/2 \ldots N\pi/2$, with $N \leq 13$) are commonly used to test for a variety of microwave-induced anomalies and frequency shifts. Specifically, frequency shifts related to the microwave spectrum, microwave leakage, and distributed cavity phase are generally investigated by the use of this method [1]–[5]. This technique may offer leverage in the detection and calibration of the aforementioned shifts. However, as has been demonstrated for the case of both microwave leakage and distributed cavity phase shifts [6], [7], the behavior of the frequency shift at high power can be quite different from that obtained with an extrapolation performed around the optimum power. Therefore, these tests must be carried out with a great deal of care and rigorous attention to the theoretical predictions.

II. Theoretical Background

The effect of spurious components in the spectrum of the microwave excitation has been analyzed by many authors [8]–[10]. A complete theory of the shifts caused by single-sideband spurs in Cs beam primary frequency standards can be found in [11] and is the basis for the analysis here. From a theoretical point of view, the analysis of the shift in frequency standards based on thermal beams and fountains is indistinguishable, with the exception that in fountain frequency standards integration over the velocity distribution is not strictly necessary. Also, the ratio of the Rabi-to-Ramsey lengths (l/L) is replaced by the ratio of the respective transit times (τ/T_R). The analytical derivation of the shift carried out in [11] is quite complete and obtained with only the approximations that each excitation has constant amplitude and that the spur power is much smaller than the optimum power or the carrier power. We recall here for the reader's convenience the main result obtained for mono-velocity atoms in [11]:

$$\delta\omega = \frac{\tau}{T_R}\frac{b_1^2}{b_0}\left(y + z_1\cos\left(\Delta T_R\right) + z_2\sin\left(\Delta T_R\right)\right), \tag{1}$$

where $\delta\omega$ is the frequency shift, τ is the interaction time inside the microwave cavity (Rabi time), T_R is the free flight time (Ramsey time), b_1 and b_0 are the Rabi frequencies of the spur and the carrier, respectively, Δ is the detuning of the spur frequency from the atomic resonance, and y, z_1, and z_2 are given by (2) (see next page). It is evident from (2) that, at those Rabi frequencies where $b_0\tau$ equals $N\pi$, the shift, given by (1), diverges. This has no particular physical meaning because at those points no microwave excitation occurs (the transition probability is zero). Fur-

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$$
\begin{aligned}
y &= \frac{1}{b_0\tau \sin(b_0\tau)} \left\{ \frac{b_0}{\Delta} \cos(b_0\tau) + \frac{1}{1-(\Delta/b_0)^2} \left(\frac{\Delta}{b_0} - \frac{b_0}{\Delta} \cos(b_0\tau)\cos(\Delta\tau) - \sin(b_0\tau)\sin(\Delta\tau) \right) \right\}, \\
z_1 &= \frac{\cos(b_0\tau)}{b_0\tau \sin^2(b_0\tau)} \frac{1}{1-(\Delta/b_0)^2} \left\{ (\cos(b_0\tau)-1)\sin(\Delta\tau) + \frac{b_0}{\Delta}(1-\cos(\Delta\tau))\sin(b_0\tau) \right\}, \qquad (2) \\
z_2 &= \frac{\cos(b_0\tau)}{b_0\tau \sin^2(b_0\tau)} \frac{1}{1-(\Delta/b_0)^2} \left\{ (1+\cos(b_0\tau))(1-\cos(\Delta\tau)) - \frac{b_0}{\Delta}\sin(b_0\tau)\sin(\Delta\tau) \right\}.
\end{aligned}
$$

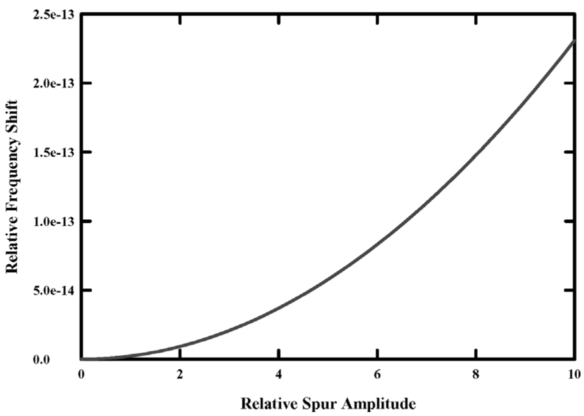

Fig. 1. The frequency shift vs. spur amplitude. A single sideband spur is assumed at 50 Hz from resonance, and unit amplitude corresponds to −40 dBc. The carrier power is fixed such that $b_0\tau = \pi/2$. Here and in most subsequent figures the Ramsey time is assumed to be 0.5 s and the Rabi time 0.01 s.

ther, even with the very narrow velocity distribution in a fountain, the Rabi frequency is not exactly the same for all of the atoms.

III. Power Dependence of the Shift

From (1), it is evident that the shift due to the presence of a spur is a quadratic function of its amplitude (linear in its power), as shown in Fig. 1. However, this statement can be misleading. Only when the ratio between the carrier power and the spur power is changed so that the carrier power remains constant will the frequency shift be proportional to the spur power. When tests at high power are performed in fountain frequency standards, the absolute power of the carrier is also usually varied. In most practical cases either the power of the spur remains constant while the carrier power is changed (this is the case when the power is varied on the IF input of a mixer, and the spur is on the LO input) or the spur varies with the carrier, maintaining the same power ratio (this is the case when the power is varied with an amplifier or an attenuator). As we will show below, the behavior of the shift is quite different in these two cases. In neither of these cases is the frequency bias induced by the spur a linear function of the microwave power. Additionally, when optimum power (defined by $b_0\tau = N\pi/2$, N being an odd integer) is perfectly set, as in Fig. 1, then the terms z_1 and z_2 in (2) are identically zero. This condition is, however, not realized in practice with the consequence that the behavior of any frequency shift as a result of spurs is considerably more complicated than that shown in Fig. 1.

While the theory of the effect of spurs contained in (1) and (2) is general, two distinct cases can be isolated, those where $\Delta \leq 1/\tau$, that is, the spur is near the Rabi excitation pedestal, and those where $\Delta \gg 1/\tau$ (the spur is well outside the Rabi pedestal). We first analyze the behavior of the shift for the case of a spur 50 Hz from the carrier, that is, near the Rabi pedestal.

We choose to study the frequency shift with excitation power in the neighborhood of optimum excitations, i.e., where the transition probability approaches unity. (This avoids the singularity in (1) at microwave powers where the transition probability approaches zero.) We find that the value of the frequency shift depends strongly both on how closely optimum microwave power is obtained and on the details of the spur frequency relative to the Rabi and Ramsey times. In Fig. 2, the value of the frequency shift caused by a spur 50 Hz from the carrier as well as one at 49 Hz, with a power −40 dBc, is shown for the cases of optimum power, optimum power ±1%, and optimum power ±2% for the lowest occurrences of unity transition probability. It is difficult to set the excitation power at optimum better than a fraction of a percent in practice, because both the atom trajectory through the microwave cavity and variations in its velocity affect the optimum microwave power. It is evident from the striking differences between these two curves that the behavior of the frequency shift is quite rich. The value of the frequency shift at high microwave excitation amplitudes is dominated by whether the microwave field is slightly above or below optimum amplitude in the case of a 50 Hz spur, whereas a very small change in the spur frequency causes the frequency shift to be essentially unaffected by small variations in the microwave field amplitude. The measured frequency shift at a given multiple of $\pi/2$ may therefore be determined mostly by the fact that the microwave power is different from optimum power and/or by the details of the spur frequency with respect to the Rabi time. Small changes in launch velocity can therefore change the frequency shift associated with a spur in a relatively large fashion. Given the apparent large sensitivity to these effects, it seems quite difficult in practice to use high-power microwave tests alone to look for frequency shifts caused by spurs in the microwave spectrum.

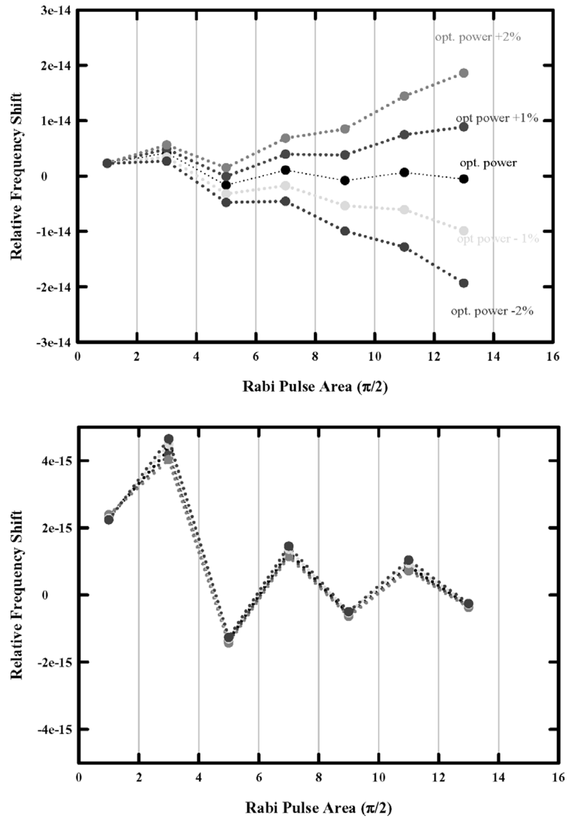

Fig. 2. Behavior of the frequency shift around optimum microwave power. In the upper graph, the spur frequency is 50 Hz, -40 dBc, whereas in the lower graph, the spur frequency has changed by 1 Hz to 49 Hz, also -40 dBc. For each optimum excitation the frequency shift is calculated for optimum excitation ($N\pi/2$) as well as $N\pi/2 \pm 1\%$ and $\pm 2\%$. The color scheme in the upper graph is carried through into the lower graph (for example, optimum excitation +2% is shown in red). The behavior of the shift is remarkably different in these two cases, thus illustrating that making unambiguous predictions of frequency shifts in real world measurement situations is, at best, difficult.

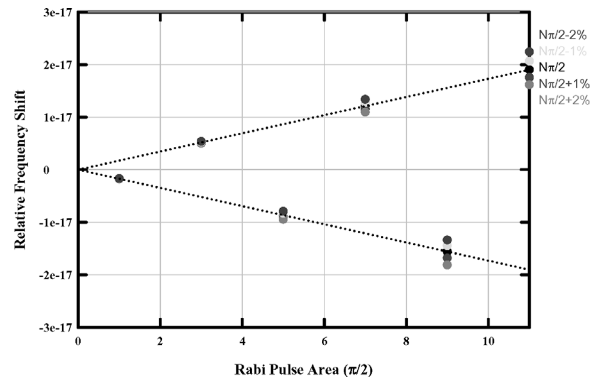

Fig. 3. Behavior of the shift around optimum excitation power. Spur: 50 kHz ($\Delta \gg 1/\tau$), -40 dBc. For each optimum power the shift is calculated for $N\pi/2$ and for $N\pi/2 \pm 1\%$ and $\pm 2\%$.

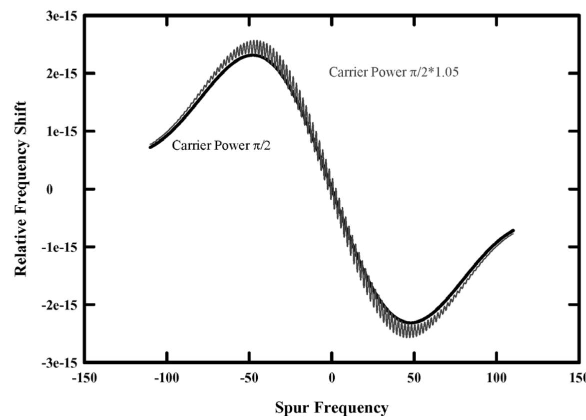

Fig. 4. Frequency shift as a function of spur frequency with excitation power at optimum and 5% above. The spur is -40 dB with respect to the carrier in both cases.

If the spur frequency is well outside the Rabi envelope, the behavior of the shift changes dramatically because the y term in (1) becomes dominant as the Ramsey structure diminishes. The period of the singularities doubles with respect to the previous case, occurring at $b_0\tau = 2N\pi$. The amplitude of the shift is inversely proportional to the detuning ($\delta\omega \propto 1/\Delta$), and the behavior shown in Fig. 2 changes to a strong oscillation in the frequency shift pattern. "Bistable" linear behavior with microwave amplitude (and not power) can be observed, as shown in Fig. 3.

We now consider the behavior of the frequency shift with respect to the spur frequency at various excitation powers. In Fig. 4 we see that, when the optimum power is precisely set, the shift is a smooth function of the frequency, whereas when this condition is not met, the shift shows Ramsey oscillations whose period is $2\pi/T_R$. This is easily understood since the phase of the atomic superposition changes with the Ramsey period, causing either a positive or a negative interference with the excess microwave phase excursion due to the spur. Averaging over even a narrow distribution of Ramsey times can easily wash out these oscillations.

At higher powers, the functional behavior can change completely. For example, when the excitation power corresponds to exactly a $5\pi/2$ pulse, we find the behavior shown in Fig. 5. If the spur power is kept constant, the modulus of the shift decreases with respect to the $\pi/2$ case. On the other hand, if the ratio between the spur and the carrier power is kept constant, the shift can be either larger or smaller in modulus depending on the spur frequency. A $\pi/2$–$5\pi/2$ test (for example) to enhance the shifting effect of a generic spurious component can therefore be meaningless unless it is carefully coordinated with the appropriate theory.

Finally, in Fig. 6, we analyze the shift caused by a spur out of resonance, when the power of the spur is kept constant, and the power of the carrier is increased to multiples of the optimum power. This case is important in many practical instances, because it corresponds to the situation where the power delivered to the atoms is varied in the last stage of the synthesis chain through the IF input of the final mixer. In this case we can see that the shift decreases by increasing the excitation power.

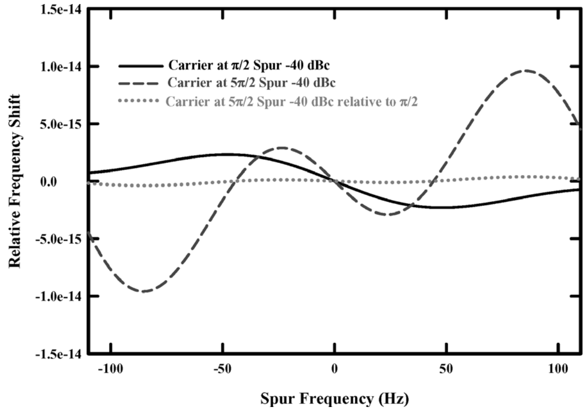

Fig. 5. Frequency shift as a function of spur frequency with excitation power at optimum ($\pi/2$) and spur -40 dBc (continuous line); carrier at $5\pi/2$, spur -40 dBc (dashed line); and carrier at $5\pi/2$ and spur -40 dBc with respect to a $\pi/2$ pulse (dotted line).

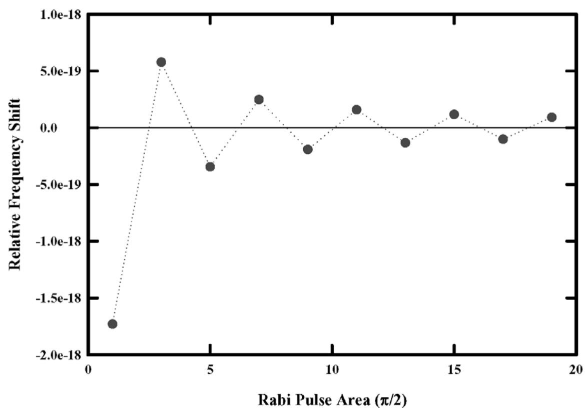

Fig. 6. Frequency shift caused by a spur at 50 kHz, -40 dBc at $\pi/2$.

IV. Experimental Results

While experimental investigations of the theory in [11] have been previously carried out in thermal beam standards [12], we have extended this to the pulsed fountain high-power regime generally inaccessible to thermal beam standards. We have made several measurements using the primary frequency standard NIST-F1 [1] which agree reasonably well with the results predicted by (1). The agreement is less than perfect for a number of reasons. The theory derived at in [11] (which we use here) assumes a constant amplitude Rabi pulse, whereas the Rabi pulse shape is a half-sine wave in the TE_{011} cavity used in NIST-F1. Unfortunately, it is not possible to derive an analytic solution similar to (1) with half-sine-wave excitation. Further, as we discuss in the next section, the theory in [11] was derived for thermal beam standards which typically have wide velocity distributions and operate continuously. This allowed the authors of [11] to average over arrival times in the microwave cavity, thereby eliminating quasi-coherent effects between the spur phase and the atom arrival time in the cavity. These effects can be quite large and are not accounted for here. We will discuss them in a future paper. With these caveats in mind, we can examine the experimental investigation of the frequency shifts predicted by (1).

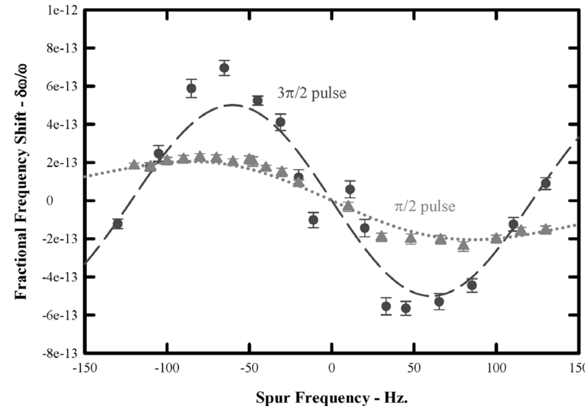

Fig. 7. Comparison between the theoretical prediction of the frequency shift (dotted and dashed lines) caused by a single sideband spur -20 dBc and experimental measurements (individual points) of the frequency shift. These data were obtained at optimum Rabi frequency ($\pi/2$ and $3\pi/2$ pulse areas) with Ramsey times of 0.565 s and Rabi times of 5.59 ms. The error bars on the experimental data are statistical.

In Fig. 7, we show the prediction and experimental data for the case of a single-sideband spur which is kept at -20 dBc while the frequency of the spur is varied. The data in red are for the case of optimum Rabi frequency so that the pulse area is $\pi/2$, whereas the data in blue are from measurements where the Rabi frequency was such that the pulse area is $3\pi/2$. All of the experimental data shown here were obtained with a Ramsey time of 0.565 s and an effective Rabi time of 5.59 ms. The theoretical curves for these conditions, as predicted by (1), compare reasonably well with the experimental data. We believe the discrepancies between the prediction and the data are mostly due to the pulsed operation of the fountain in the case of the $\pi/2$ data whereas both these effects and small misadjustments of the Rabi frequency are probably apparent in the $3\pi/2$ data. The shape of the excitation profile inherent in the theory is different from the experimental excitation profile which is most evident at spur detunings larger than half the Rabi width ($\sim$15 Hz).

While important effects for pulsed operation are not included in the original theory of [11], it is clear that the predictions of that theory are at least qualitatively correct when the spur detuning frequency is carefully chosen to avoid coherent effects between the detuning frequency and the cycle time of the fountain, as is the case for the data presented here. These coherent effects are discussed further in the next section.

V. Pulsed Operation

Because most fountain frequency standards operate in the pulsed regime, it is worthwhile to examine the consequences of pulsed operation. If we consider the time-

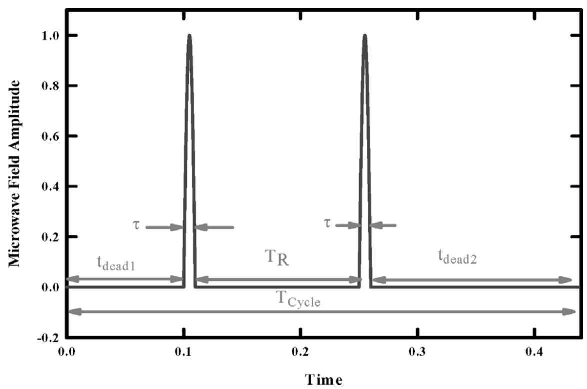

Fig. 8. Amplitude modulation of the microwave power, as seen by the atoms, during a fountain cycle.

domain picture of the microwave field as seen by the atoms, it is generically similar to that shown in Fig. 8. The microwave field is zero until the atom enters the Ramsey cavity. It turns on smoothly to a maximum and then turns off smoothly back to zero over a time τ (the Rabi time). The microwave field is then zero for a time T_R (the Ramsey time) at which point the microwave field again turns up smoothly to a maximum and then back to zero. This pattern is then repeated for each cycle of operation.

Suppose an unwanted pure frequency modulation at frequency ω_1 is present on the carrier. The extraneous phase introduced by this modulation can be written as

$$\beta \cos \omega_1 t, \tag{3}$$

where β is the modulation index ($\beta = \Delta f / f_1$, where Δf is the frequency deviation produced by the frequency modulation). We assume that the atoms are centered in the cavity on the way up at t_1 and again on the way down at $t_2 = T_R + t_1 + \tau$, where $t = 0$ is taken as the launch time. The change in phase between the two interactions due to the modulation is then given by

$$\delta\varphi = \beta \left[\cos \omega_1 t_2 - \cos \omega_1 t_1\right] = \\ -2\beta \sin \omega_1 \left(t_1 + \frac{1}{2} T_R + \frac{1}{2}\tau\right) \sin \omega_1 \left(\frac{1}{2} T_R + \frac{1}{2}\tau\right). \tag{4}$$

Associated with this phase difference is a frequency shift of order $\delta\varphi / T_R$. N fountain cycles later the phase difference would be the same, with t_1 augmented by NT_{cycle}. As long as $\omega_1 T_{\text{cycle}}$ is not an integer times π (or an integer times a rational fraction of π), this phase difference and any accompanying shift will average to zero after many fountain cycles. But if, for example, the modulation frequency is 50 Hz and the cycle time is exactly 1.020 s (51 cycles at 50 Hz), the same phase difference will occur during each fountain cycle and the associated shift will persist.

From a frequency point of view, the microwave spectrum effectively has all of the harmonic components that are multiples of $1/T_{\text{cycle}}$. If one of these spectral components is coincident with a component of the frequency modulated spectrum, it will produce an asymmetric sideband. Hence, balanced sidebands present in the synthesizer can cause frequency shifts, because the pulsed operation of the fountain automatically generates sidebands that may interfere. We are presently conducting further investigations into these quasi-coherent effects.

VI. Conclusions

It is clear that the perception that the frequency shift caused by a spur in the microwave spectrum is quadratic in its amplitude is, at best, an oversimplification in practical cases that apply to fountain frequency standards. Given the extremely complex behavior of the frequency shifts caused by the presence of spurious components in the microwave excitation spectrum, we conclude that high-power microwave tests need to be carefully analyzed by comparison with appropriate theory. In general, no leverage can be expected with experiments carried out at higher excitation power. The amplitude and sign of the shift can vary widely, depending on the spur frequency, the Rabi-pedestal width, the Ramsey time, and whether the microwave power is slightly above or below optimum. It is therefore very difficult to correct for shifts related to spectral components. This difficulty is compounded by the pulsed operation and possible synchronicity between the spur frequency and the fountain cycle time. Therefore, to guarantee a given level of accuracy in a fountain frequency standard, we must estimate the maximum ratio of acceptable spur to carrier in the spectrum, and ensure that this ratio has been met with independent measurements. For example, assume that a fountain is operated with $T_R = 0.5$ s and $\tau = 0.01$ s and must be accurate at $\delta\nu/\nu_0 = 10^{-16}$ level. A spur within the Rabi pedestal must be reduced to almost -60 dBc. For a spur far off resonance, the constraints are more relaxed because larger detunings allow higher spur powers. For example, a spur 50 kHz from the carrier can be -20 dBc and still allow an accuracy of 1×10^{-16}.

Acknowledgments

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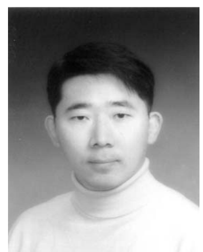

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