Microwave Leakage-Induced Frequency Shifts in the Primary Frequency Standards NIST-F1 and IEN-CSF1

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***Abstract*—In atomic fountain primary frequency standards, the atoms ideally are subjected to microwave fields resonant with the ground-state, hyperfine splitting only during the two pulses of Ramsey's separated oscillatory field measurement scheme. As a practical matter, however, stray microwave fields can be present that shift the frequency of the central Ramsey fringe and, therefore, adversely affect the accuracy of the standard. We investigate these uncontrolled stray fields here and show that the frequency errors can be measured, and indeed even the location within the standard determined by the behavior of the measured frequency with respect to microwave power in the Ramsey cavity. Experimental results that agree with the theory are presented as well.**

I. Introduction

All Cs primary frequency standards are based on Ramsey's separated oscillatory field technique. The atoms pass once through a microwave cavity in which they interact with a resonant microwave field. They then proceed in a free-flight zone in which nominally no microwave field is present. They finally pass through a second microwave cavity in which the Ramsey excitation process is completed. After a short free flight, the atoms are detected. This description is valid for both the laser-cooled fountains and the thermal beams, even if the practical realization of these devices is quite different. In fact, in a laser-cooled fountain, the atoms are launched upward (typically at $\sim$5 m/s) and are decelerated to a stop by gravity before retracing the (nominally) same trajectory on the way down. Hence, in this kind of frequency standard, only one cavity is necessary to implement the two-zone excitation. In a beam experiment, two cavities are placed at a certain distance apart along the beam path to provide the two-zone excitation.

A certain level of microwave leakage always is present in frequency standards. The effects of such leakage were previously investigated, both experimentally and theoretically [1]–[3]. Possible frequency biases resulting from microwave leakage are typically evaluated by applying elevated microwave excitation power [4]–[7]. We show that the shifts have a complex oscillatory dependence on excitation power. The details depend critically on the location of the leakage within the standard, complicating the use of elevated microwave power as a diagnostic.

The atoms can interact with leakage microwave fields at three distinct times. First, the atoms can be irradiated between state-selection and the first Ramsey interaction. Second, the atoms can be irradiated with leakage microwaves in the free-flight region, that is, between the two Ramsey pulses. Third, the atoms can be irradiated by leakage microwave fields between the second Ramsey interaction and the detection region. All three types of microwave leakage can be analyzed by the same basic theoretical formulation. This formulation is a slight extension of that developed for the distributed cavity phase shift [8]. The theory will be described in the next section and applied to the three cases. Simple leakage models will be presented to illustrate the dependence on excitation power.

In general, it is extremely difficult to give a precise model of the leakage field because its phase and amplitude can vary with multiple reflections in the laboratory environment and is unlikely to be stable in time. In the Appendix of the paper, however, we will numerically solve a particular case in which the drift region is within a cylindrical multiwavelength TE_{11N} cavity. This model applies to both NIST-F1 and IEN CsF1, respectively the fountain primary frequency standards of the National Institute of Standards and Technology, Boulder, CO, and of the Istituto Elettrotecnico Nazionale "G. Ferraris," Torino, Italy, because the drift tube above the Ramsey cavity is below cutoff for all modes, except the fundamental TE_{11} mode of a cylindrical waveguide. Because the drift tube is terminated at each end by a waveguide below cutoff for the fundamental mode, the distribution (but not phase) of any leakage field is calculable in this particular case.

II. Schrödinger Equation Formulation and Ramsey Lineshapes

We extensively used the theoretical framework developed by Shirley *et al.* [9]–[11] and give here the extensions required to handle the out-of-phase but on-frequency (with

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respect to the cavity field) quadrature component of the leakage microwave field.

We begin by assuming that the problem can be handled within the framework of a two-level system. The Hamiltonian for the system can be written as (cf. (7) of [11])

$$H = \hbar \begin{pmatrix} \omega_a & 2b\cos\omega t + 2b'\sin\omega t \\ 2b\cos\omega t + 2b'\sin\omega t & \omega_b \end{pmatrix}, \quad (1)$$

where $\hbar\omega_a$ and $\hbar\omega_b$ are, respectively, the energies of the upper and lower states. The interaction Rabi frequency for the in-phase or real part of the microwave field is given by $2b = \mu_B g \operatorname{Re}(H_Z)/\hbar$, where μ_B is the Bohr magneton, g is the Landé g-factor, and H_Z is the microwave magnetic field parallel to the quantization axis imposed by the external C-field. Similarly, the Rabi frequency for the quadrature or imaginary part of the microwave field is given by $2b' = \mu_B\, g\operatorname{Im}(H_z)/\hbar$. Both $b(t)$ and $b'(t)$ may be time dependent owing to the atoms' motion in the leakage field.

In the rotating wave approximation, the Hamiltonian (1) is written:

$$H = \hbar \begin{pmatrix} \omega_a & (b+ib')e^{-i\omega t} \\ (b-ib')e^{i\omega t} & \omega_b \end{pmatrix}. \quad (2)$$

Note the sign change in $b'(t)$ in the off-diagonal couplings. This comes about because the rotating-wave approximation selects one exponential from $\sin\omega t$ in one coupling and the other exponential in the other coupling (Compare to (7) and (8) in [11]). This sign change retains Hermiticity of the Hamiltonian. By using "phase factored" probability amplitudes, the exponential time dependence of the off-diagonal elements in (2) can be transformed to a constant contribution to the diagonal elements (cf (9) and (10) of [11]). The resulting Schrödinger equation for the system is:

$$i\hbar\frac{d}{dt}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \hbar\begin{pmatrix} -\Delta & (b+ib') \\ (b-ib') & \Delta \end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}. \quad (3)$$

Here, Δ is half the detuning $\delta\omega$ from the atomic resonance ω_0: $\Delta = \frac{1}{2}(\omega - \omega_0) = \frac{1}{2}\delta\omega$, in which $\omega_0 = \omega_a - \omega_b$ is the hyperfine splitting of the atom. $\mathit{\Delta}$, b, and b' are all real.

We impose the initial conditions $\alpha(0) = 1$ and $\beta(0) = 0$. Then α is the probability amplitude that the system remains in its initial state, and β is the probability amplitude that the system changes state.

If we write out the real and imaginary parts of the equations in (3) we have four coupled equations in four real variables. When b' is zero and the initial conditions in (3) hold, we see that $\operatorname{Re}\alpha$ and $\operatorname{Im}\beta$ are even functions of the detuning $\mathit{\Delta}$, and $\operatorname{Im}\alpha$ and $\operatorname{Re}\beta$ are odd functions. The transition probability, which is the sum of the squares of the real and imaginary parts of β, is thus an even function of detuning and, hence, centered on the resonance. This remains true independent of the time dependence that b may have. We could consider $b(t)$ to include the Ramsey excitation and the leakage fields. But, as long as all the fields are in phase there is no shift. The effect of in-phase leakage is merely an alteration in the amplitude of the Ramsey fringes. The presence of the quadrature component b' destroys this detuning symmetry, allowing frequency shifts to occur. In the following we have set the phase of the microwave field in the Ramsey cavities to zero, and we will consider only the quadrature leakage component b' as we look for shifts.

We first give a solution to (3) for the excitation regions. We assume b' and $\mathit{\Delta}$ are small enough to be neglected compared to the excitation Rabi frequency. The solution of (3) is then (compare (25)–(28) of [11]):

$$\begin{aligned}\alpha(\tau) &= \cos b_0\tau, \text{ and}\\ \beta(\tau) &= -i\sin b_0\tau,\end{aligned} \quad (4)$$

where $b_0\tau = \int_0^\tau b(t)dt$, that is, b_0 is the average value of $b(t)$ during the excitation time τ.

For the leakage region, we denote the Rabi frequencies and corresponding probability amplitudes by a subscript L. We consider only the case of $b'_L/b_0 \ll 1$. To first order α_L is not affected. Hence, we find the approximate solution to (3):

$$\begin{aligned}\alpha_L(t) &= e^{i\Delta t},\\ \beta_L(t) &= -e^{-i\Delta t}\int_0^t b'_L(t')e^{2i\Delta t'}dt'.\end{aligned} \quad (5)$$

Without a specific form for the magnitude and phase of the microwave leakage field experienced by the atom, we cannot evaluate the integral for β_L. However, in the case of a constant amplitude for the leakage field applied for a time t_L, the solution (5) becomes:

$$\begin{aligned}\alpha_L(t_L) &= e^{i\Delta t_L},\\ \beta_L(t_L) &= -\frac{b'_L}{\Delta}\sin(\Delta t_L).\end{aligned} \quad (6)$$

This result for constant excitation will be used throughout this paper as a test case that allows us insight into the physics of the problem. If Δt_L is sufficiently small, (6) reduces to $\alpha_L = 1$ and $\beta_L = -b'_L t_L$. Any spatial form of leakage field always can be approximated with an arbitrary degree of accuracy by a series of constant excitations of varying b'_L and t_L because, as we stated previously, the in-phase term, b, cannot cause frequency shifts.

III. Microwave Leakage After the Ramsey Excitation

As our first example, we consider that the microwave leakage takes place after the second Ramsey interaction. If we use subscripts 1 and 2 to denote the first and second Ramsey microwave interactions and denote the Ramsey drift time by T_R, the wave function for Ramsey excitation can be written as (compare (35) of [11]):

$$\psi(t_L + \tau_2 + T_R + \tau_1) = \begin{pmatrix}\alpha_L & -\beta_L^*\\ \beta_L & \alpha_L^*\end{pmatrix}\begin{pmatrix}\alpha_2 & -\beta_2^*\\ \beta_2 & \alpha_2^*\end{pmatrix}\begin{pmatrix}e^{i\Delta T_R} & 0\\ 0 & e^{-i\Delta t_R}\end{pmatrix}\begin{pmatrix}\alpha_1 & -\beta_1^*\\ \beta_1 & \alpha_1^*\end{pmatrix}\psi(0), \quad (7)$$

where $\psi(0)$ is given here by:

$$\psi(0) = \begin{pmatrix} \alpha(0) \\ \beta(0) \end{pmatrix} \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (8)$$

The form of the evolution matrices is dictated by unitarity. The transition amplitude from the initial state to the final state then is given by:

$$\beta\left(t_L + \tau_2 + T_R + \tau_1\right) = \left(\beta_L \alpha_1 \alpha_2 + \alpha_L^* \alpha_1 \beta_2\right) e^{i\Delta T_R} + \left(\alpha_L^* \alpha_2^* \beta_1 - \beta_L \beta_1 \beta_2^*\right) e^{-i\Delta T_R}, \quad (9)$$

where the subscripts refer to the first and second pass through the Ramsey cavity. We can simplify (9) by substituting our approximate solutions (4) for $\alpha_{1,2}$ and $\beta_{1,2}$, assuming that the two passes through the Ramsey cavity are the same. We obtain:

$$\beta\left(t_L + \tau_2 + T_R + \tau_1\right) = -i \sin 2b_0\tau \cos \Delta T_R \alpha_L^* + \left(\cos 2b_0\tau \cos \Delta T_R + i \sin \Delta T_R\right) \beta_L.$$

For a simplest approximation we insert (6) and get the approximate transition probability,

$$P = \frac{1}{2} \sin^2\left(2b_0\tau\right)\left[1 + \cos\left(\delta\omega T_R\right)\right] + b_L' t_L \sin\left(2b_0\tau\right) \sin\left(\delta\omega T_R\right). \quad (10)$$

We have assumed Δt_L is small because in fountains the leakage time after excitation will be much less than the drift time, due to the greater atom velocity. The first terms in (10) represent the normal Ramsey fringe lineshape. The last term in (10), proportional to the quadrature part of the leakage b_L', represents Ramsey fringes out of phase with the normal Ramsey fringes. It is the cause of the frequency shift associated with the leakage.

If slow, square-wave modulation of the applied frequency is used to observe the Ramsey resonance, we measure (10) on the left and right sides of the central fringe at detunings $-\omega_{\text{mod}}$ and ω_{mod}, respectively. The difference $P_L - P_R$ between these measurements constitutes the error signal used to steer the tuning of the excitation frequency. For (10) the error signal becomes:

$$P_L - P_R = 2b_L' t_L \sin\left(2b_0\tau\right) \sin\left(\omega_{\text{mod}} T_R\right). \quad (11)$$

It has a dependence on the excitation power through b_0 such that it is maximum at optimum power, but alternates in sign as power increases beyond the first optimum. The actual frequency shift is given by dividing the error signal (11) by the difference in the slope of the Ramsey fringe on the left and right sides of the fringe. The result is:

$$\delta\omega = \frac{2b_L' t_L}{T_R \sin 2b_0\tau}, \quad (12)$$

assuming the shift is small compared to the fringe spacing. From (10) $\delta\omega_L$ is bounded by $\pi/2T_R$. A distribution of excitation times τ also will bound the shift. The apparent divergence when $2b_0\tau = \pi$ is a mathematical artifice because the signal vanishes there. However, because this divergence tends to dominate plots of the actual frequency shift versus $b_0\tau$, we have chosen to plot the error signal (11) rather than the frequency shift in most of the figures presented here.

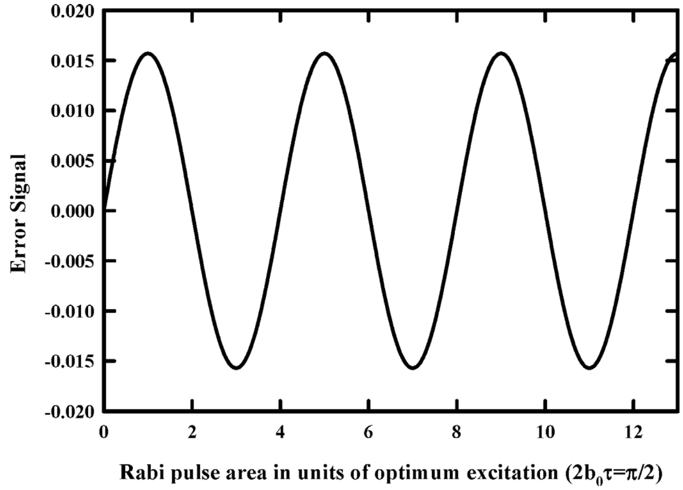

Fig. 1. The error signal caused by microwave leakage after the second Ramsey pulse. The strength of the leakage field is 10^{-2} of optimum power, and the leakage is applied with a phase shift of $\pi/2$ relative to the field in the Ramsey cavity.

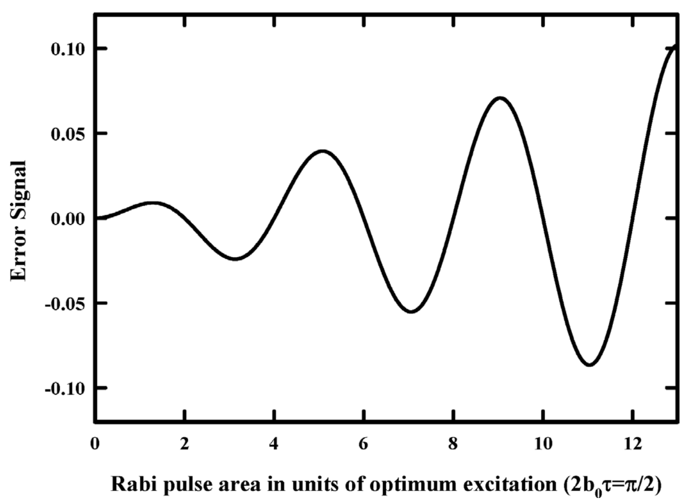

Fig. 2. The error signal caused by microwave leakage after the second Ramsey pulse when the strength of the leakage field is proportional to the field in the Ramsey cavity.

The error signal (11) caused by constant-amplitude microwave leakage between the second Ramsey pulse and optical detection is illustrated in Fig. 1. In the case of NIST-F1 and IEN-CSF1, the amplitude of the leakage field after the second Ramsey pulse is likely to be proportional to the excitation microwave field applied to the atoms. In that case, the error signal created by the microwave leakage is of the approximate form $\delta\nu \propto b_0\tau \sin\left(2b_0\tau\right)$ as shown in Fig. 2. The error signal due to leakage after the Ramsey cavity can be very difficult to separate from the error signal due to distributed cavity phase [8] as a result of the very similar "signature" of the two effects, as illustrated in Fig. 3.

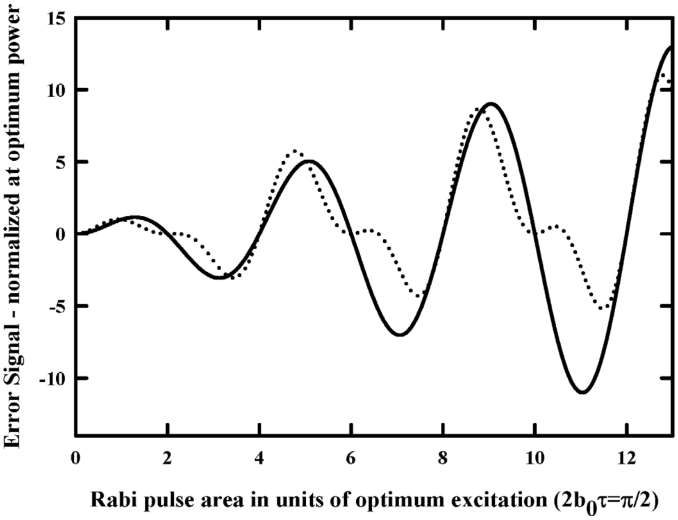

Fig. 3. The error signal from leakage after the second Ramsey interaction (solid line) compared with the error signal caused by distributed cavity phase (dotted line). These may be quite difficult to separate experimentally!

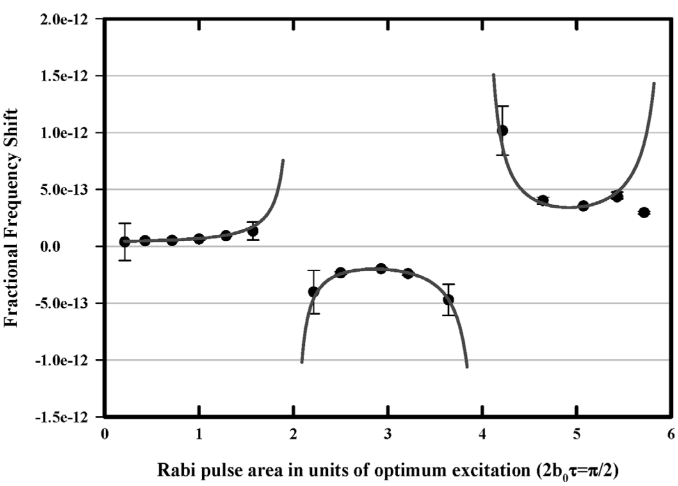

Fig. 4. The frequency error induced by leakage after the second Ramsey interaction. The solid curve is the result of (12). The data are measured (using NIST-F1) for the case in which a small amount of microwave energy from the Ramsey synthesizer was deliberately coupled into the state-selection microwave cavity that lies between the Ramsey cavity and the atom detection zone.

We have experimentally investigated microwave leakage after the second Ramsey interrogation by coupling a small amount of energy from the microwave synthesizer that drives the Ramsey microwave cavity into the state-selection microwave cavity directly below the Ramsey cavity. In Fig. 4 we show a comparison between the predictions of the theory presented here (solid curve) and measured frequency shifts (single points) for the case in which the leakage amplitude is proportional to the Ramsey excitation amplitude. The theoretical fit is a plot of (12). The overall magnitude of the fitted shift was adjusted because, although we can control the amplitude of the leakage, the phase of the leakage is unknown though stable. This adjustment is made so that the theoretical prediction and the experimental result coincided at the lowest Ramsey excitation amplitude. The agreement is quite good, except at the highest excitation amplitudes in which second order effects, not included within our theory, begin to become important. The error bars on the data points are purely statistical in nature, and the relatively large error bars for some data are a result of the microwave amplitude being close to that for no net excitation.

IV. Microwave Leakage Before the Initial Ramsey Excitation

In this case, the leakage evolution matrix in (7) will come before the excitation matrices. In place of (9), we then find the transition amplitude:

$$\beta\left(\tau+T+\tau+t_L\right)=\left(\beta_2\alpha_1\alpha_L-\beta_2\beta_1^*\beta_L\right)e^{i\Delta T_R}+\left(\alpha_2^*\beta_1\alpha_L+\alpha_2^*\alpha_1^*\beta_L\right)e^{-i\Delta T_R}.$$

Under the same assumptions used in deriving (10), we obtain the transition probability:

$$P=\frac{1}{2}\sin^2\left(2b_0\tau\right)\left[1+\cos\left(\delta\omega T_R\right)\right]-b_L' t_L\sin\left(2b_0\tau\right)\sin\left(\delta\omega T_R\right).$$

The only difference between this result and (10) is the sign of the leakage correction term. Hence, we have the same qualitative results and power dependence of the leakage error signal. Note that, if the leakage before excitation is the same as the leakage after excitation, the net leakage error vanishes.

In some fountains and in NIST-F1 and IEN-CSF1 in particular, there can be no leakage before excitation because the atoms are within a below-cutoff waveguide between state-selection and the first Ramsey interaction. Thus, the atoms entering the Ramsey cavity from below in these particular fountains are in a pure $F=3$, $m_F=0$ state.

V. Microwave Leakage Between the Two Ramsey Excitations

In this case (7) is rewritten as

$$\psi\left(\tau_2+T_R+\tau_1\right)=\begin{pmatrix}\alpha_2 & -\beta_2^*\\ \beta_2 & \alpha_2^*\end{pmatrix}\begin{pmatrix}e^{i\Delta T_R} & -\beta_L^*\\ \beta_L & e^{-\Delta T_R}\end{pmatrix}\begin{pmatrix}\alpha_1 & -\beta_1^*\\ \beta_1 & \alpha_1^*\end{pmatrix}\psi(0), \quad (13)$$

where $\alpha_L$has been replaced by $e^{i\Delta T_R}$. We shall retain the detuning dependence in β_L because the leakage time may be comparable to T_R. The transition amplitude is then:

$$\beta\left(\tau_2+t_L+\tau_1\right)=\beta_2\alpha_1 e^{i\Delta T_R}+\alpha_2^*\beta_1 e^{-i\Delta T_R}+\alpha_2^*\alpha_1\beta_L-\beta_2\beta_1\beta_L^*.$$

Substituting from (4) this reduces to:

$$\beta\left(\tau_2+T_R+\tau_1\right)=-i\sin 2b_0\tau\cos\left(\Delta T_R\right)+\operatorname{Re}\beta_L+i\cos 2b_0\tau\operatorname{Im}\beta_L.$$

The resulting transition probability becomes:

$$P = \frac{1}{2}\sin^2 2b_0\tau\,[1+\cos(\delta\omega T_R)] - 2\sin 2b_0\tau\cos 2b_0\tau\cos\left(\delta\omega T_R/2\right)\operatorname{Im}\beta_L(T_R), \quad (14)$$

plus terms quadratic in β_L. From (5) we have:

$$\operatorname{Im}\beta_L(T) = -\int_0^T b_L'(t)\sin(2\Delta t - \Delta T_R)\,dt. \quad (15)$$

This integral is an odd function of detuning, so it may cause a shift. But note that the argument of the sine is an odd function of $t - T_R/2$. Hence, if b_L' is an even function of $t - T_R/2$, such as a constant value, the integral and associated shift vanish.

The leakage term in (14) vanishes at optimum power, that is, where $2b_0\tau = \frac{1}{2}(2n+1)\pi$, $n = 0, 1, 2, \ldots$. It also changes sign twice as frequently as the corresponding term due to leakage before or after Ramsey excitation. This difference in power dependence helps to distinguish the different cases of leakage.

As an example of a case in which an error occurs, we consider leakage applied at constant amplitude and phase during the first half of the Ramsey drift time, that is, until the atoms reach apogee. From apogee until the second Ramsey interaction, we consider the leakage field to be zero. This case contains all the fundamental physics of the problem and illustrates the behavior of the error signal with increasing power in the Ramsey excitation (e.g., $-\frac{\pi}{2}$, $\frac{3\pi}{2}$, etc.). Inserting this artificial dependence into (15) we find:

$$\operatorname{Im}\beta_L(T_R) = \left(b_L'/\Delta\right)\sin^2\left(\Delta T_R/2\right).$$

We substitute this result into (14) in the case of slow square-wave frequency modulation to obtain the error signal

$$P_L - P_R = -\frac{2b_L'}{\omega_{\rm mod}}\sin(4b_0\tau)\cos\left(\omega_{\rm mod}T_R/2\right)\left[1-\cos\left(\omega_{\rm mod}T_R/2\right)\right]. \quad (16)$$

This error signal is plotted in Fig. 5 as a function of the excitation power in units of optimum power ($2b_0\tau = \pi/2$) with the modulation amplitude set to one-fourth of a fringe spacing. This model of leakage is somewhere between unlikely and impossible in the real world, but the frequency error associated with leakage above the cavity will, in general, have the structure shown in Fig. 5. The model used here affects the size of the error, but not its shape (modulo a factor of -1). As stated earlier, if the microwave field seen by the atoms is symmetric with respect to $T_R/2$, the frequency bias vanishes, but perfect symmetry is unlikely in the real world in which fountain tilts and ballistic expansion of the atomic sample generally will cause the symmetry condition to be violated to some degree. Another effect related to the lack of symmetry caused by ballistic expansion and fountain tilts recently was pointed out in [12].

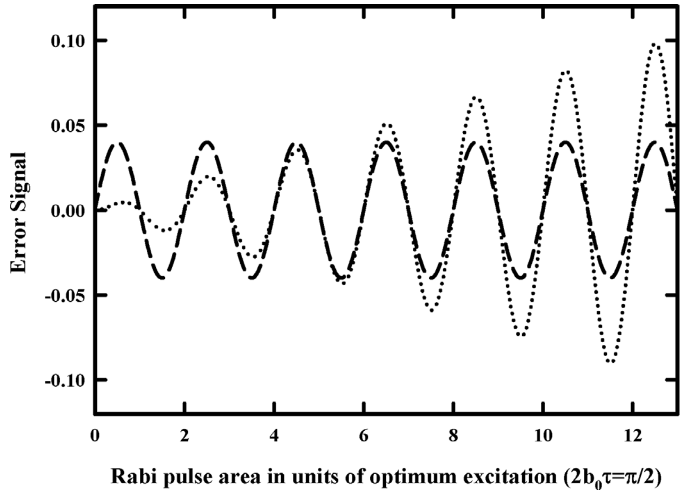

Fig. 5. The effect of leakage between the two Ramsey excitations on the error signal. The dashed line is the case in which the leakage field amplitude is independent of Ramsey excitation strength. The dotted curve, which grows with increasing Ramsey excitation, is for the case where $b_L' \propto b_0$. The relative size of the leakage fields shown here was chosen for clarity and has no other significance.

That effect, caused by unequal Rabi pulses on the two transits of the Rabi cavity, may or may not be dominant, depending on the details of the fountain and laser-cooling involved. However, the symmetry condition is largely met in cesium fountains, with the result that leakage above the Ramsey cavity typically causes small, frequency shifts unless the leakage field is quite large. In the case in which the field is quite large, second order effects are likely to be important, especially at elevated microwave powers.

We have numerically integrated the Schrödinger equation with $b_L = b_L'$ for the range of Ramsey excitations such that $0 \le b_0\tau \le 11\pi/2$. The numerical work did not make all the approximations made in the theory. But the results agree well with Fig. 5.

We also have experimentally investigated the case of leakage above the Ramsey cavity. This was done by using the microwave cavity directly below the Ramsey cavity (normally used for state selection) as the Ramsey cavity and coupling a small amount (-28 dB) of the microwave energy into the cavity usually used for Ramsey excitation. These "leakage" microwaves were turned on only during the first passage of the atoms through the "leakage" microwave cavity. Data obtained using this system are shown in Fig. 6. The dashed line is the frequency shift predicted from (16) divided by twice the slope of the Ramsey curve at $\pm\omega_{\rm mod}$; and the data are shown as single points. The error bars are purely statistical. The theoretical curve, $\delta\omega \propto b_L' ctn\,(2b_0\tau)$, is fit to the data with two adjustable parameters. These parameters scale the amplitude of the leakage field, b_L' and the amplitude of the field in the "Ramsey" cavity, b_0. As can be seen, the agreement between the theoretical prediction and the corresponding measurement is quite good. This ideal experimental situation approximates the case of NIST-F1 and IEN-CsF1 quite well because any leakage above the Ramsey cavity is a (essentially pure) standing wave (see the Appendix).

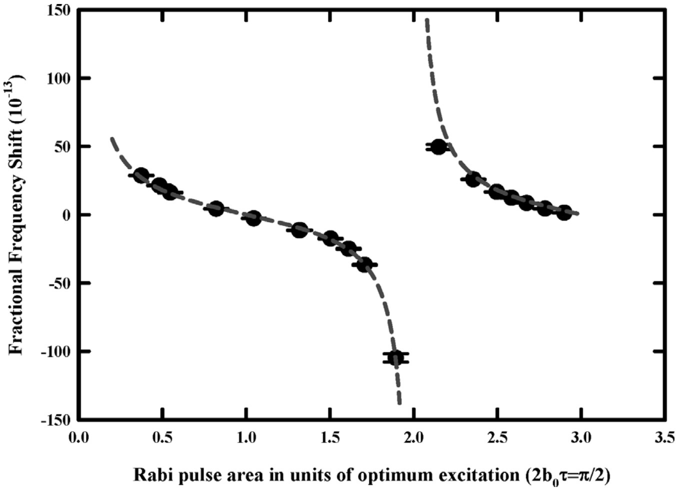

Fig. 6. The frequency error induced by leakage between the two Ramsey interactions. The dashed curves are the theoretical prediction [embodied in (16)]. The data are measured (using IEN-CSF1) for the case in which a small amount of microwave energy from the Ramsey synthesizer was deliberately coupled into the upper microwave cavity. The lower cavity, usually used for state selection, was used instead for Ramsey excitation.

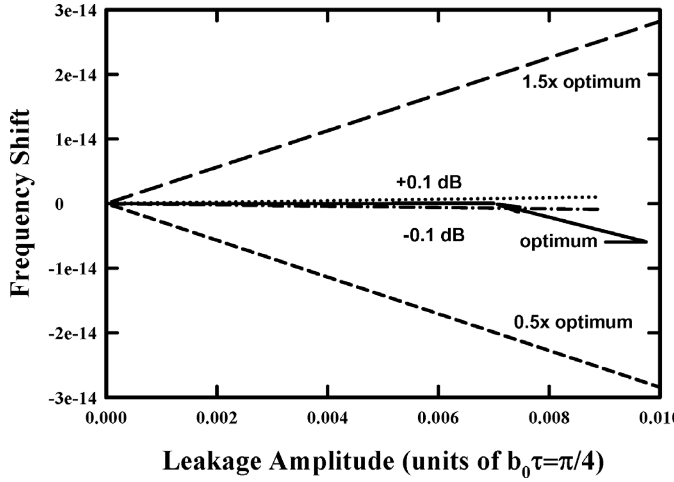

Fig. 7. The frequency error caused by microwave leakage between the two Ramsey pulses. The error is very small at optimum power but can be enhanced by deliberately operating at nonoptimum microwave power in the Ramsey cavity. The size of the frequency error shown here was simply chosen for convenience and carries no particular application to any given apparatus.

While the fountain was in this configuration, we also allowed the microwaves to remain on for both passes of the atom cloud. In this case, the theory predicts no frequency shift (assuming perfect atomic-trajectory retrace). Indeed, the frequency shift was suppressed by a factor of more than 20 compared to the single pass experiment. The residual shift demonstrates the effects of imperfect atomic retrace caused by atom temperature and possible fountain tilt. See also [12] and [13].

To search for a frequency error due to microwave leakage above the Ramsey cavity of a fountain, one can make measurements well above and below optimum power, as illustrated in Fig. 7. In NIST-F1 the microwave power is set to within ±0.1 dB of optimum, denoted by the dotted lines in Fig. 7. The frequency error induced by microwave leakage (leakage proportional to $b_0\tau$) with $b_0\tau = 1.5$ and 0.5 times optimum excitation is some 30 times greater than the error expected within 0.1 dB of optimum. For detecting an error, measurement at 1.5 and 0.5 times optimum excitation, therefore, gives a "leverage" of 30 compared to standard operating conditions. This leverage, of course, assumes that the amplitude of any microwave leakage is strictly proportional to the amplitude of the microwave field within the Ramsey microwave cavity, that the leakage field is small enough so second order effects are negligible, and that the effects of imperfect retrace are small. These assumptions may or may not be valid, depending upon the specific circumstances that apply to the measurement. This measurement only measures the effect of leakage above the Ramsey cavity, which in many cases will cause smaller frequency biases than leakage below the Ramsey cavity. The error budget for microwave leakage in both NIST-F1 and IEN-CSF1, for example, is dominated by the effects of microwave leakage below the cavity.

VI. Discussion

We have shown that a frequency bias is introduced by the microwave leakage field only if certain conditions are met. First, the leakage field must have a component out-of-phase with respect to the microwave field within the Ramsey cavity. Second, this leakage field, as experienced by the atoms, must have an antisymmetric component with respect to the midpoint of the Ramsey free flight time. The presence of a quadrature phase component to the microwave field is the same requirement found for the distributed cavity phase shift in primary frequency standards [8].

The power dependence of frequency errors attributable to microwave leakage in fountain-type frequency standards is quite complicated. Oscillations in the sign of the frequency bias occur at powers far above optimum, and the period of these oscillations depends on the location of the leakage (above or below the Ramsey cavity). As we have shown here, the power dependence of the error signal also is critically dependent upon the location of the leakage within the standard. In the case of leakage between the two Ramsey interactions, the error signal is minimized at optimum power; but when the leakage is either before or after the Ramsey interaction, the leakage causes a maximum error signal at optimum power in the Ramsey cavity.

The theory we present is strictly applicable only in the case of resonant interaction between the leakage microwaves and the atoms. However, the maximum Doppler shift of the leakage in a typical cesium fountain is of the same order as the Rabi width (∼100 Hz) and under these conditions the theory remains qualitatively correct and is quantitatively correct within a factor of 2, see [2] and [12]. In NIST-F1 and IEN-CSF1, the leakage above the Ramsey cavity is always resonant because, as explained in the Appendix, the drift tube is a high Q, antiresonant microwave cavity. The leakage below the Ramsey cavity is described by a combination of standing (dominant) and traveling waves with Doppler shifts of as much as 100 Hz.

The dependence on microwave power of the error signal caused by microwave leakage either before or after the Ramsey interaction and the error signal caused by distributed cavity phase are very similar, as illustrated in Fig. 3. This can cause these two effects to be difficult to separate experimentally. However, the effects can be lumped together, and a limit on the frequency error due to either source can be obtained by measuring the frequency bias as a function of microwave field within the Ramsey cavity. It also may be possible to modulate any leakage either in amplitude or frequency in order to distinguish the frequency bias from this source from that caused by distributed cavity phase.

Given that the accuracy of cesium fountain frequency standards is now $\delta f/f \leq 10^{-15}$, frequency errors from microwave leakage must be kept to the $\delta f/f = 10^{-16}$ level or below. This means that the microwave leakage field in a typical fountain must be less than about -130 dB relative to the field in the Ramsey cavity (the precise statement is $(b' t_L / 4 T_R b_0 \tau) \leq \delta\nu$).

It should be noted that there are various methods to avoid microwave leakage. The group at Bureau National de Metrologie Systemes de Reference Temps-Espace (BNM-SYRTE) have developed a dark-fringe microwave interferometric switch that they use to turn on and off the microwaves delivered to the frequency standard without introducing a phase error [14]. This is a powerful method, but it requires very careful microwave engineering to avoid phase errors at the microradian level. It also is possible to frequency-modulate the microwaves delivered to the fountain so that any leakage field is off resonance with the hyperfine splitting of the atoms, thus reducing and changing the frequency error associated with the leakage [15]. Both of these methods suffer from the fact that the modulation, be it AM or FM, is, by necessity, synchronous with the fountain cycle and any phase-transients induced on the Ramsey-interrogation microwave field lead to frequency errors from spurs very close to the carrier that can be quite difficult to detect.

As a result of the unstable nature of microwave leakage in a normal laboratory environment, it always is preferable to eliminate the source of the leakage rather than trying to correct for it.

Appendix A
A Leakage Model for NIST-F1 and IEN-CSF1

In NIST-F1 and IEN-CSF1, we are fortunate to have a relatively simple system to analyze in determining the leakage microwave fields above the Ramsey cavity. We begin by describing the physical system.

The Ramsey cavity is 6.00 cm in diameter and 2.2 cm high, and operated in the TE_{011} mode. Above the Ramsey cavity is a 10-cm long, 1-cm diameter copper tube that acts as a below cutoff waveguide for the microwave field within the Ramsey cavity. Above the below-cutoff waveguide is a 2.5-cm diameter copper tube about 85-cm long. The copper tube allows propagation of the TE_{11} mode, with the next lowest frequency mode, the TM_{01} being just at cutoff. At the top of the copper drift tube is a 5-cm long section of 304 stainless-steel tubing with a vacuum seal window. The inner diameter of this tube is 1.75 cm; thus, this tube is below cutoff for all modes at 9.193 GHz. The dominant TE_{11} mode has an attenuation of 36 dB in this 1.75-cm diameter tube, and the next mode, the TM_{01}, an attenuation of 84 dB, some 48 dB more than the TE_{11} mode. The field within the drift region of the fountain, therefore, is predominantly TE_{11}, and its source is leakage down the 5-cm long stainless tube. The drift region thus forms a TE_{11N} cavity in which N must be determined. The mode number N is between 33 and 34, that is, the cavity length is somewhere between 33/2 and 34/2 guide wavelengths long where:

$$\lambda_g = \frac{2\pi}{\beta}, \text{ and } \beta = \sqrt{k_0^2 - \left(\frac{\rho'_{1,1}}{r_D}\right)^2}, \text{ with}$$
$$k_0 = \frac{\omega_0}{c} \text{ and } \rho'_{1,1} \simeq 1.841. \tag{17}$$

The guide wavelength, λ_g is 5.06 cm at 9.193 GHz in a copper tube with $r_D = 1.25$ cm as used here. Therefore, the leakage field is given (to first order) by a superposition of the $TE_{1,1,33}$ and $TE_{1,1,34}$ modes with the relative amplitudes a function of the frequency detuning of 9.193 GHz from the actual mode frequencies of modes 33 and 34. We therefore can write the z-component of the microwave magnetic field as:

$$H_Z = \left[\frac{H_0}{K}\right]\left[J_1\left(\frac{\rho'_{1,1} r}{r_D}\right) \times \cos\phi\left(A_{33}\sin\frac{33\pi(z-12.2)}{\lambda_g} + A_{34}\sin\frac{34\pi(z-12.2)}{\lambda_g}\right)\right], \tag{18}$$

where $\rho'_{1,1}$ is defined as the first solution of $dJ_1(x)/dx = 0$ and A_{33} and A_{34} are the relative amplitudes of the two TE_{11} modes of the drift tube in question. K is an attenuation factor and, as used in (18), is much greater than 1. The origin of the z-coordinate is taken at the bottom edge of the Ramsey cavity.

The relative amplitudes of modes 33 and 34 can be quickly evaluated with the help of the following picture. The Q for each mode, evaluated using the known resistivity of copper, is given by:

$$Q_{1,1,N} = \frac{\lambda_0}{\delta_S}\frac{\left[1-\left(\frac{1}{\rho'_{1,1}}\right)^2\right]\left[\left(\rho'_{1,1}\right)^2 + \left(\frac{N\pi r_D}{L}\right)^2\right]^{3/2}}{2\pi\left[\left(\rho'_{1,1}\right)^2 + \frac{2r_D}{L}\left(\frac{N\pi r_D}{L}\right)^2 + \left(1-\frac{2r_D}{L}\right)\left(\frac{N\pi r_D}{\rho'_{1,1} L}\right)^2\right]}. \tag{19}$$

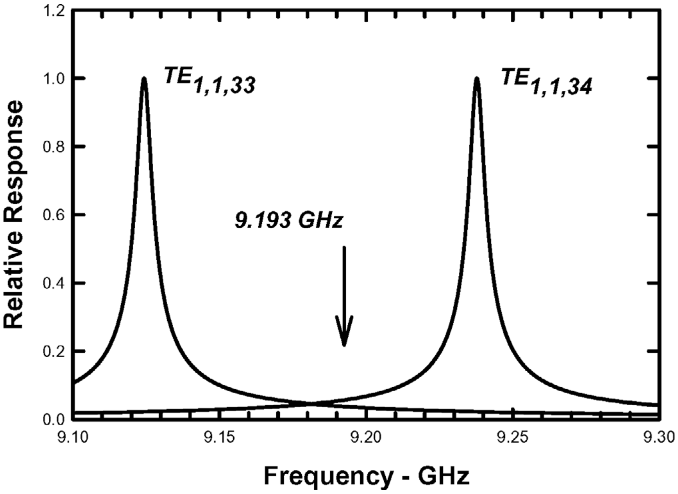

Fig. 8. The relative response of the 33 and 34 modes. Note that, in the figure, the Q is degraded by a factor of 100 in order to make the resonance width broad enough to be seen.

In (19) λ_0 is the free-space wavelength, L is the cavity length, and $\delta_S = \sqrt{2/\omega\mu\sigma}$ ($\approx$ 0.7 μm for the copper used here) is the skin depth in the material, where μ and σ are the permeability and conductivity of the material ($\mu \simeq 4\pi \times 10^{-7}$ and $\sigma \simeq 5.8 \times 10^7$ S/m for copper). The Q then evaluates as approximately 1.8×10^4 for both modes. The relative excitation for each mode is then given by evaluating the overlap of modes 33 and 34 with the 9.193 GHz drive frequency. The resonant frequencies for modes 33 and 34 are 9.12 GHz and 9.24 GHz, respectively. The amplitude of excitation of the mode versus frequency is given by:

$$A_{33} \propto \frac{1}{\left[4\left(\omega_{33}-\omega\right)^2 + \frac{\omega_{33}^2}{Q_{33}^2}\right]^{1/2}} \text{ and,}$$
$$A_{34} \propto \frac{1}{\left[4\left(\omega_{34}-\omega\right)^2 + \frac{\omega_{34}^2}{Q_{34}^2}\right]^{1/2}}, \tag{20}$$

here ω_{33} is $(2\pi)f_{33}$, the resonant frequency for mode 33 with a similar expression for ω_{34}. Also Q_{33} is the quality factor of mode 33 and similarly for Q_{34}. The physical interpretation of A_{33} and A_{34} is the height of the response function for these modes at the 9.1926 GHz drive frequency as illustrated in Fig. 8. Because the drift tube length is antiresonant at 9.1926 GHz, the leakage field in the drift tube is strongly attenuated in NIST-F1 and IEN-CSF1.

The microwave fields seen by the atom as a function of z, therefore, are given by:

$$\begin{aligned} H_z &= \left(\frac{\pi H_0}{2}\right) J_0\left(\frac{\rho'_{0,1}\rho}{r_C}\right)\sin\left(\frac{\pi z}{d}\right), \ d = 2.2 \text{ cm and} \\ &\quad 0 \le z \le 2.2 \text{ (inside the Ramsey cavity)}, \\ H_z &= 0 \text{ for } 2.2 \le z \le 12.2 \text{ (inside the below-cutoff} \\ &\quad \text{waveguide)} \\ H_z &= \text{Eq. (18) and (20) for } z \ge 12.2 \text{ cm (inside the} \\ &\quad \text{drift tube)}. \end{aligned} \tag{21}$$

We have numerically integrated the Schrödinger equation using (21) as the leakage field with the phase arbitrarily set to be $\pi/4$ with respect to the field in the Ramsey cavity. The same integration code was extensively tested against the various leakage types we have solved analytically; the numerical results agreed well with the analytic results in all cases. In the numerical solution using the field given in (21), the atoms are assumed to have a thermal velocity $\nu_X = \nu_Y = \nu_Z = \sqrt{kT/m}$ and a density distribution equal to the measured density distribution in NIST-F1. K in (18) is set to 10^4 and the excitation in the Ramsey cavity is swept from 0 to $11\pi/2$. Under these conditions, the excitation has an asymmetric part as a result of the steadily changing radial positions of the atoms, and the resulting error signal is essentially identical to that shown in Fig. 5.

For a cloud of atoms with an atom density distribution symmetric about the drift tube axis, the frequency bias is zero in this particular case. This occurs because the atoms average over the $\cos\phi$ dependence of the TE_{11} mode in the drift tube. We have been unable to measure any frequency error associated with leakage above the Ramsey cavity in our fountains without introducing extremely large microwave fields so the second order effects (not discussed here, see [2] and [12]) become significant.

In NIST-F1 the microwave synthesizer [13] allows us to change the Ramsey excitation amplitude from $2b_0\tau = 0.5 \times (\pi/2)$ to $2b_0\tau = 1.5 \times (\pi/2)$ by changing only the amplitude of the 7 MHz signal reaching the final mixer for which the 9193 MHz Ramsey interrogation signal is generated. This mixer is well terminated at all ports. The output amplitude of the microwave synthesizer is quite linear with respect to the amplitude of the 7 MHz, with the amplitude of the 7 MHz required for an excitation of $3\pi/2$, $5\pi/2$, and $7\pi/2$ being 3, 5, and 7 times (respectively) the amplitude required for a $\pi/2$ excitation. All elements of the signal path between the final mixer and the Ramsey cavity are linear (e.g., splitters, attenuators, and circulators). There are no physical changes to the microwave system when making this measurement (the system is untouched). Therefore, the amplitude of any microwave leakage should be strictly proportional to b_0, allowing us to perform the leveraged tests searching for frequency shifts caused by microwave leakage above the Ramsey cavity discussed earlier (see Fig. 7). We have measured this error signal in NIST-F1 and find a possible frequency shift from this term with $\delta f/f \le 5 \times 10^{-17}$. It should be noticed that this test is only for leakage above the Ramsey cavity; we test for leakage below the Ramsey cavity using the theory that results in (12). In NIST-F1, the frequency uncertainty associated with leakage below the Ramsey cavity is dominant.

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References

[1] K. Dorenwendt and A. Bauch, "Spurious microwave fields in caesium atomic beam standards: Symmetry considerations and model calculations," in *Proc. Eur. Time Freq. Forum*, 1999, pp. 57–61.

[2] B. Boussert, G. Théobald, P. Cérez, and E. deClercq, "Frequency shifts in cesium beam clocks induced by microwave leakages," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 45, pp. 728–738, 1998.

[3] W. D. Lee, J. P. Lowe, J. H. Shirley, and R. E. Drullinger, "Microwave leakage as a source of systematic error and long-term instability in cesium atomic beam frequency standards," in *Proc. Eur. Time Freq. Forum*, 1994, pp. 513–516.

[4] S. R. Jefferts, J. Shirley, T. E. Parker, T. P. Heavner, D. M. Meekhof, C. Nelson, F. Levi, G. Costanzo, A. DeMarchi, R. Drullinger, L. Hollberg, W. D. Lee, and F. L. Walls, "Accuracy evaluation of NIST-F1," *Metrologia*, vol. 39, pp. 321–336, 2002.

[5] S. Weyers, U. Hübner, R. Schröder, C. Tamm, and A. Bauch, "Uncertainty evaluation of the atomic caesium fountain CSF1 of the PTB," *Metrologia*, vol. 38, pp. 343–352, 2001.

[6] F. Levi, L. Lorini, D. Calonico, and A. Godone, "IEN-CSF1 accuracy evaluation and two-way frequency comparison," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, pp. 1216–1224, 2004.

[7] K. Szymaniec, W. Chalupczak, P. B. Whibberley, S. N. Lea, and D. Henderson, "Evaluation of the primary frequency standard NPL-CsF1," *Metrologia*, vol. 42, pp. 49–57, 2005.

[8] S. R. Jefferts, J. H. Shirley, N. Ashby, E. A. Burt, and G. J. Dick, "Power dependence of distributed cavity phase induced frequency biases in atomic fountain frequency standards," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 52, no. 12, pp. 2314–2321, 2005.

[9] J. H. Shirley, "Some causes of resonant frequency shifts in atomic beam machines I. Shifts due to other frequencies of excitation," *J. Appl. Phys.*, vol. 34, pp. 783–788, 1963.

[10] J. H. Shirley, "Solution of the Schrödinger equation with a Hamiltonian periodic in time," *Phys. Rev.*, vol. 138, pp. B979–B987, 1965.

[11] J. H. Shirley, W. D. Lee, and R. E. Drullinger, "Accuracy evaluation of the frequency standard NIST-7," *Metrologia*, vol. 38, pp. 427–458, 2001.

[12] S. Weyers, R. Schröder, and R. Wynands, "Effects of microwave leakage in caesium clocks: Theoretical and experimental results," in *Proc. Eur. Time Freq. Forum*, 2006.

[13] S. R. Jefferts, J. H. Shirley, N. Ashby, T. P. Heavner, E. A. Donley, and F. Levi, "On the power dependence of extraneous microwave fields in atomic frequency standards," in *Proc. IEEE-UFFC Freq. Contr. Symp.*, 2005, pp. 105–110.

[14] M. Abgrall, "Evaluation des Performances de la Fontaine Atomique PHARAO, Participation à l'étude l'horloge spatiale PHARAO," Ph.D. dissertation, University de Paris VI, Paris, France, Jan. 2003. (in French)

[15] T. P. Heavner, S. R. Jefferts, E. A. Donley, T. E. Parker, and F. Levi, "A new microwave synthesis chain for the primary frequency standard NIST-F1," in *Proc. IEEE Freq. Contr. Symp.*, 2005, pp. 308–311.

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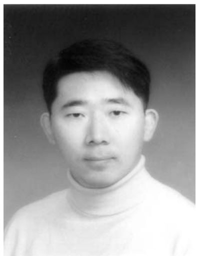
Since 2003 he has worked as a researcher at INRIM, where he is involved with laser-cooled atomic frequency standards in the microwave and in the optical domain.



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