PHYSICS OF SYSTEMATIC FREQUENCY VARIATIONS IN HYDROGEN MASERS

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ABSTRACT

The frequency stability of hydrogen masers for intervals longer than 10^4 seconds is limited at present by systematic processes. We discuss the physics of frequency-determining mechanisms internal to the maser that are susceptible to systematic variations, and the connections between these internal mechanisms and external environmental factors. Based upon estimates of the magnitudes of systematic effects, we find that the primary internal mechanisms currently limiting long-term maser frequency stability are cavity pulling, at the level of parts in 10^{15} per day, and wall shift variations, at the level of parts in 10^{16} to parts in 10^{15} per day. We discuss strategies for reducing systematic frequency variations.

INTRODUCTION

The hydrogen maser is the most stable frequency standard currently available, providing fractional frequency stabilities of better than 1×10^{-15} for averaging intervals on the order of 10^4 seconds. The fundamental mechanisms limiting maser frequency stability are well know: additive thermal noise entering the maser's r.f. receiver¹ causes the two-sample (Allan) deviation $\sigma(\tau)$ to vary with the averaging interval τ as τ^{-1} , and is the dominant mechanism typically for $\tau < 100$ seconds, while thermal noise within the atomic linewidth² causes $\sigma(\tau)$ to vary as $\tau^{-1/2}$, and typically dominates the stability for $100 < \tau < 10^4$ seconds³. For intervals longer than roughly 10^4 seconds, $\sigma(\tau)$ generally increases with τ , due to systematic processes affecting the frequency. In this regime, typical plots of the Allan deviation show $\sigma(\tau) \sim \tau^1$, indicating domination by linear frequency drift. When linear drift is removed from the frequency data, $\sigma(\tau)$ often varies as $\tau^{1/2}$, which is characteristic of random-walk of frequency. Random walk frequency variations are likely to result from the simultaneous action of several quasi-independent processes; an underlying $\tau^{1/2}$ variation of $\sigma(\tau)$ suggests that a number of systematic effects are at work in addition to the dominant long-term process.

In order to improve the long-term frequency stability of hydrogen masers, systematic frequency-varying processes must be identified and reduced. At the present level of maser performance, not one, but many such processes must be dealt with in order to achieve a substantial improvement in long-term stability. The aim of the present work is three-fold: first, to identify sources of systematic frequency variation; second, to estimate the magnitudes of the various combinations of effects on the frequency stability; and third, to identify strategies for minimizing these systematic effects.

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SOURCES OF SYSTEMATIC FREQUENCY VARIATION

The sources of systematic frequency variation in hydrogen masers can be organized into three groups, as shown in Table. 1: (i) the basic internal mechanisms that determine the maser's frequency⁴, including cavity pulling, internal magnetic fields and field gradients, wall shift, collisional frequency shifts, and second order Doppler effect; (ii) environmental variables, including ambient temperature, magnetic field, humidity, barometric pressure, vibration, gravity, and time; and (iii) the myriad structures and systems within the maser that can connect, or transduce, environmental changes to the internal mechanisms. Time is included as an environmental or driving mechanism because many components, both mechanical and electronic, are observed to vary slowly, or "age," without direct external intervention.

Table 1 — Schema of Frequency-determining Mechanisms				
Maser Frequency Physics (Internal)		Driving Mechanisms (External)		
Cavity frequency (pulling) Magnetic field (internal) Wall shift Collisional shifts 2nd Order Doppler shift (dPhase/dt)	←Transducing← Mechanisms	Time Temperature Magnetic field (external) Humidity Vibration Barometric pressure Gravity		

Transducing mechanisms, and their connections between environmental drivers and internal maser physics, are listed in Table 2. As indicated in Table 2, the links between environmental and internal mechanisms are multiple, with many environmental drivers acting upon several physical mechanisms, often through several different transducing effects, and many internal mechanisms affected by more than one environmental force. Because all active masers necessarily employ systems that accomplish similar ends, the list of transducers is relatively general; the magnitudes of systematic frequency variations, however, can differ by orders of magnitude, depending upon the specifics of maser design.

Relevant to practical considerations of maser frequency stability, but not included in the list of Table 2, are noise and phase variations introduced by the comparison system used to measure maser frequencies. Thermal and mechanical disturbance of signal-carrying cables, and thermal noise in amplifiers and mixers, can introduce phase changes that are difficult to separate from maser frequency variations; these effects are most important in relatively short-term comparisons (under 30 minutes), and will be particularly important when comparing cryogenic masers, which are projected to have stabilities in the range of 10^{-17} to 10^{-18} .

Internal	Transducing Mechanism	Time	Temp	Humid	Baro	MagFld	Vib
Mechanism	<u> </u>		-				
Cavity Frequency	Bulb Dielectric coef		X				
	Cavity bulk thermal		X				
	expansivity						
	Cavity coating thermal		X				
	expansivity						
	Tuning diode voltage	?	X	?			
	Cavity joint shrinkage	X					<u>X</u>
	Cavity bulk shrinkage	X					
	Coupling circuit/isolator	?	X	??			
	Thermistors/resistors	X					
	Beam flux variation	?	X	?			
	Barometric pressure				X		
						· · · · · · · · · · · · · · · · · · ·	
Magnetic Field	External mag fld variation	X				X	
magnitude &	Internal field current var.		X				
gradients	Magnetic shield aging	?					X
	Atomic state distribution						
Wall Shift	Storage bulb	X					
	contamination						
	Coating changes	X					
	·····						
Collisional Shifts	State distrib. changes	?	?			X	
	Beam flux variation	?	X				
2nd order	Temperature		X				
Doppler			·				

Table 2 — Connections Among Frequency-determining Mechanisms

Some of the transducing effects of Table 2 require explanation. An important internal maser frequency-determining mechanism is cavity pulling: a change Δf_c of the maser's resonant cavity frequency produces a change Δf_m in the maser frequency given by

$$\Delta f_c = \Delta f_m (Q_c / Q_{\text{line}}) \tag{1}$$

where Q_c is the loaded cavity Q and Q_{line} is the atomic line Q. The main factor affecting the cavity's resonance frequency is the cavity's size: the resonance frequency of a typical cavity varies with cavity length at a rate of roughly 10 MHz/cm, so that for $Q_c/Q_{line} \sim 10^{-5}$, a typical value, a fractional change in the maser frequency of 10^{-15} , which is readily measurable, is produced by a cavity length change of roughly one Angstrom, or the size of an atom. The cavity's dimensions are affected by the thermal

expansivity α of the material of which the cavity is constructed ($\alpha \sim 10^{-8} \circ C^{-1}$ for low-expansion materials like Cervit or Zerodur, and $\alpha \sim 2 \times 10^{-5} \circ C^{-1}$ for metals such as copper or aluminum); contraction of the joints between the cavity's cylinder and endplates over periods of months to years⁵; thermal expansivity of the cavity's metallic coating (for non-metallic cavity materials); change in the coating's internal stress⁶; and shrinkage of the cavity's (bulk) structural material over years^{7,8,9}. The cavity's resonance frequency is also affected by thermally-induced changes in the quartz storage bulb's dielectric coefficient and by changes in the cavity's varactor tuning diode voltage, which can result from temperature changes in the diode voltage reference or voltage divider circuit (or digital-to-analog converter [DAC], if used), and from aging of the reference, divider, or DAC.

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Internal magnetic fields affect the maser's frequency primarily through the quadratic dependence of the hydrogen hyperfine energy upon magnetic field, and also, in masers that are not properly tuned, through magnetic-gradient line broadening, which can change the amount of cavity pulling by varying the line Q. In addition, the internal field affects the magnetic gradient shift¹⁰, which depends upon the d.c. magnetic field gradient, asymmetry in the r.f. magnetic field, and the state distribution in the atomic beam. Variations in the internal magnetic field can result from changes in the external (ambient) magnetic field, which is never perfectly excluded by the maser's magnetic shields; from changes in the shielding factor of the shields that may result from vibration or, possibly, from aging; and from changes in the current that supplies the solenoid that generates the uniform internal field. The solenoid current is susceptible to many of the environmental mechanisms that can affect the tuning diode voltage.

Slow changes in maser frequency due apparently to variations in the wall shift have been observed. Wall shift changes might be caused by contamination of the storage surface by materials outgassed from other parts of the maser or entering the storage bulb from the hydrogen dissociator; by outgassing of contaminants from the bulb surface (cleanup); and by physical or chemical changes in the fluorocarbon storage coating itself.

Frequency shifts due to collisions between stored hydrogen atoms — spin-exchange shifts and so-called Crampton-Verhaar shifts — are affected by variations in the hydrogen beam flux intensity and by changes in the magnetic fields in the region between the state-selection magnets and the resonant cavity, which can vary the distribution of atomic states entering the storage bulb.

The second-order Doppler shift affects the maser frequency directly through the speed, and therefore the temperature, of the hydrogen atoms in the storage bulb.

ESTIMATION OF SYSTEMATIC EFFECTS

APPROACH TO ESTIMATION

In estimating the magnitude of the many frequency-varying effects, both analytical and experimental approachs are used. Some effects can be analysed from physical principles; for example, the second-order Doppler shift Δf_D is directly related to the temperature of the storage bulb, while the change in the cavity resonance frequency due to cavity expansion can be expressed as a

function of the cavity's temperature and the cavity material's thermal expansion coefficient α . Other effects are difficult or impossible to analyse from first principles, and must be measured; examples are cavity joint shrinkage, and cavity frequency changes resulting from variation in the length of the coaxial cable coupling the cavity to the r.f. output circuit. Some effects, such as magnetic field sensitivity or thermal variations, can be measured in controlled, relatively short-term tests; others, notably the wall shift and cavity shrinkage, require very long-term observations and measurements.

For all effects, estimating absolute frequency variations requires assumptions about the construction of the maser, the effectiveness of its control systems, and the magnitudes of environmental variations. Here we assume an active maser with a low-expansivity resonant cavity; thermal control that maintains the maser's cabinet air temperature constant to 0.1 °C and the cavity temperature constant to 2×10^{-5} °C; and passive magnetic shields with a shielding factor S = $\Delta H_{ext}/\Delta H_{int} \sim 4 \times 10^4$. As discussed in a later section, cavity autotuning and other environmental control mechanisms, which are not assumed here, have the potential of significantly reducing some systematic frequency variations.

DISCUSSION OF SPECIFIC EFFECTS

<u>Cavity coupling circuit</u>. In addition to being a function of internal mechanisms such as the bulb dielectric coefficient and the cavity's dimensions, the cavity's resonance frequency is affected by the external circuit that couples r.f. power out of the cavity. Because the circuit terminator, usually a ferrite isolator, cannot be perfectly matched to its input coaxial cable, changes in the cable's length can alter the amount of r.f. power reflected back to the cavity, and consequently change the cavity frequency. As shown in Fig. 1, which represents measurements using a particular isolator, cable, and cavity coupling coefficient, the sensitivity of maser frequency to cable length can be as much as several parts in 10^{12} per cm if the cable's length is not adjusted optimally, or nominally zero if the cable's length is properly chosen. The choice of cable length affects not only the maser's sensitivity to the cable itself, but also its sensitivity to changes in the terminating isolator. This effect may play a part in the sensitivity to changes in ambient humidity, discussed below.

Cavity dimension changes The cavity resonance frequencies of many masers increase monotonically with time. Figure 2 shows the change in maser frequency due to cavity resonance frequency variations in Smithsonian Astrophysical Observatory (SAO) masers over periods of up to ten years¹¹. The data were obtained from the variations in the tuning diode voltages required to keep the maser cavities spin-exchange tuned¹², and were translated to a common origin for ease of comparison. The frequencies almost invariable increase, at rates that generally decrease with time, and lie between roughly 2×10^{-15} /day and 7×10^{-15} /day. A possible source of such behavior has been suggested to be shrinkage of the polished, although not optically contacted, joints between the cavity cylinder and endplates. Optically contacted joints in similar materials have been shown to shrink at roughly exponentially decreasing rates, with characteristic times on the order of months⁵. The continuing increase in cavity frequencies over many years, however, suggests shrinkage of the bulk cavity material itself. Such shrinkage has been observed in gauge-blocks of Zerodur⁷ and ULE⁹ and in Zerodur and ULE laser etalons⁸, and is summarized in Table 3. Column 3 of the table gives the equivalent maser frequency change that would result from the material shrinkage, assuming

 $Q_c/Q_{line} \sim 10^{-5}$. The substantially lower shrinkage rate observed in a ULE etalon provides reason to believe that a proper choice of cavity material can result in a significant decrease in cavity frequency variation.

Table 3 — Shrinkage Rates of Low-expansivity Cavity Materials					
Material		Material creep (1/L)(dL/dt) (day ⁻¹)	Maser freq change (1/f)(df/dt) (day ⁻¹)		
Zerodur ¹	initial	-1.8×10^{-9}	3.6×10^{-14}		
	after 10 yrs	-2.9×10^{-11}	5.8×10^{-16}		
Zerodur ²	initial ³	-3.9×10^{-10}	7.6×10^{-14}		
	after 900 days	-1.8×10^{-10}	3.6×10^{-15}		
ULE ²	initial	-3.7×10^{-9}	9.3 × 10-15		
	after 20 days	-4.6×10^{-11}	9.2×10^{-16}		
¹ Ref. 7. ² Ref. 8. ³ 1.5 years after heat treatment					

Wall Shift Even after changes in cavity frequency are accounted for by spin-exchange tuning. masers are observed to have long-term frequency drifts that are generally ascribed to changes in the wall shift. Figure 3 shows the frequencies of 7 hydrogen masers measured after tuning¹³. (The tunings and frequency measurements were generally done after the masers had been opened to the atmosphere for changing of their vacuum pump elements.) The tuned maser frequencies were compared with UTC by means of GPS common-view measurements or, in the case of the early measurements, transportable cesium clocks. (For this reason the early measurements have relatively large uncertainties.) The frequencies of most of the masers decrease with time, at rates between roughly -6×10^{-16} /day to -2×10^{-15} /day. Some of the more recently built masers, on the other hand, appear to increase slightly in frequency, at rates of up to $+6 \times 10^{-16}$ /day. These wall shift changes may be due to chemical or physical alterations in the coating materials, or to adsorption or desorption of contaminants. In addition, wall shift changes have been observed that result from changes in the hydrogen flux intensity entering the storage bulb. Wall shift variations cannot be removed by cavity retuning or servo control, and represent what is likely to be the dominant systematic effect on longterm maser frequency stability. Research into improved wall coating materials is called for, building upon Soviet work that has yielded coatings with up to 10 times less wall shift than previous materials¹⁴.

<u>Gravity</u> Gravity affects the frequency of the hydrogen maser both through the relativistic effects to which all clocks are subject, and through deformations of the maser's structure, primarily the microwave cavity. In particular, many masers are sensitive to tilt; the measured sensitivity of one maser¹⁵, for example, is 3.6×10^{-14} /degree. While tilt sensitivity should not affect the frequency stability of a maser located on a solid, it does limit the resettability of a maser after being moved, and requires masers to be carefully repositioned or retuned after being moved.

<u>Humidity</u> High-stability cesium and hydrogen clocks have been observed to be sensitive to humidity. Changes in humidity might affect a maser's frequency by altering the thermal conductivity of the air within the maser cabinet and thus affecting its temperature control systems, or by altering the surface conductivity of the high-impedance circuits supplying the tuning diode voltage; there is also evidence suggesting that humidity may affect the maser's output isolator or coaxial coupling cable¹⁶.

SUMMARY OF RESULTS

The results of measurements and calculations of a variety for systematic effect are summarized in Fig 4. The black lines give ranges of sensitivities for effects that can be estimated with a reasonable degree of confidence; gray lines represent values for which precision is lacking, or for which parameters, such as cavity detuning, can vary over a substantial range and depend upon specific maser operation. Lack of space prevents presentation of detailed derivations; details are available elsewhere¹⁷. It can be seen from Fig. 4 that, under the assumptions made here, the major systematic contributions to maser frequency variation arise from dimensional aging of the cavity material and from wall shift variation, contributing frequency variations on the order of parts in 10^{16} /day. A variety of other effects are expected to come into play at the level of parts in 10^{16} , and as a matter of observation, frequency stabilities currently appear limited, even after removal of linear frequency drift and rate of change of drift, to several parts in 10^{15} for periods of days to weeks³.

STRATEGIES FOR REDUCING SYSTEMATIC FREQUENCY VARIATIONS

A variety of approaches to reducing systematic frequency variations in hydrogen masers have been implemented or proposed. Cavity pulling in active masers has been addressed by means of servo systems that lock the cavity's resonance frequency to the atomic masing frequency^{18,19,20}. Active servo control has also been applied to the reduction of magnetic field effects; one such system concentrates and senses the magnetic field within the outermost magnetic shield and controls a solenoid to compensate for ambient field changes¹⁹. Single-state hydrogen beam state selection systems^{21,22,23} can improve magnetic performance as well as reduce cavity pulling. By preventing hydrogen atoms in undesired hyperfine states from entering the storage region these systems reduce spin-exchange relaxation, thereby increasing the line Q and decreasing cavity pulling; in addition, they substantially reduce collisional frequency shifts that make the maser susceptible to magnetic field variations²⁴.

Electronic control systems and servos, including the temperature, hydrogen flux, tuning diode, and magnetic field controllers used in all masers, are potentially subject to long-term changes due to aging of components such as voltage references, thermistors, setpoint resistors, varactor diodes, and isolators. The effects of such aging on maser frequency stability has not been reported, and will require lengthy and careful investigation to quantify.

Wall shift variations cannot be reduced by incorporating new maser systems, but rather by improving the chemical and physical properties of the wall coating material, and perhaps by identifying and reducing contaminating materials in the maser.

A different approach to improving maser frequency stability is available for use with masers that are employed as medium-term flywheel oscillators or frequency references. The drift rate of a maser can be established by spin-exchange tuning the maser at intervals of weeks to months, or by comparing the maser's frequency with international references by means of GPS common-view measurements. Using a phase-continuous digital synthesizer in the maser receiver system, the output frequency of the maser receiver can be varied in steps of less than 10^{-17} to compensate for the maser drift. The tuning diode is then reset at intervals of weeks to months to the tuned cavity condition, at which time the synthesizer frequency is adjusted simultaneously to keep the maser's output frequency constant.

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CONCLUSIONS

At the present state of the art, hydrogen maser frequency stability appears limited to a few parts in 10^{15} for intervals of days to weeks. Improvement of long-term stability will require careful attention to a variety of systematic effects. An advantageous approach to dealing with these effects appears to be to identify and reduce systematic processes as much as possible, and then to employ active servo control systems to reduce them further, taking care that the control systems do not, themselves, introduce other systematic variations.

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Fig. 3. Variation in tuned maser frequency as a function of time



Fig. 4. Summary of estimated systematic frequency variations.