Methods for Constraining Fine Structure Constant Evolution with OH Microwave Transitions

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We investigate the constraints that OH microwave transitions in megamasers and molecular absorbers at cosmological distances may place on the evolution of the fine structure constant $\alpha = e^2/\hbar c$. The centimeter OH transitions are a combination of hyperfine splitting and lambda doubling that can constrain the cosmic evolution of α from a *single species*, avoiding systematic errors in α measurements from multiple species which may have relative velocity offsets. The most promising method compares the 18 and 6 cm OH lines, includes a calibration of systematic errors, and offers multiple determinations of α in a single object. Comparisons of OH lines to the HI 21 cm line and CO rotational transitions also show promise.

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Introduction.—Recent measurements of the fine structure constant $\alpha = e^2/\hbar c$ claim a smaller value of α in the past of order $\frac{\Delta\alpha}{\alpha_\circ} \sim -10^{-5}$ at $z = 1$–2 [1,2]. Unification theories that require extra compact dimensions predict variations in the fundamental constants over cosmic time, including the fine structure constant (see [1] for a review). New physics is being developed to account for the observed properties of the Universe, such as the dark energy manifested in the cosmological constant, and these theories can be tested by high precision observations of the evolution of α over cosmic time. Murphy *et al.* [1] have called on the community to produce independent measurements of the fine structure constant evolution to verify current results from quasar absorption lines. We present a method to exploit the hyperfine structure of the OH molecule to bypass the systematic pitfalls of other radio and submillimeter determinations of $\alpha(z)$.

Centimeter OH transitions can be observed at cosmological distances in absorption against strong radio continuum sources or in OH megamasers (OHMs) [3,4]. OHMs are luminous natural masers found in the nuclei of major galaxy mergers. OHMs are luminous, can be observed with high spectral resolution, and like OH absorbers can be narrow and spatially compact, marking with high precision a specific position and redshift which reduces potential systematic errors. The frequency shift in the main 18 cm OH lines due to a change in α is considerable: $\sim$30 kHz for $\frac{\Delta\alpha}{\alpha_\circ} = 10^{-5}$. Resolution of such a shift is trivial for typical observations of OH lines; the main difficulty lies in identifying the true redshift of a given galaxy because all lines may be influenced by a changing fine structure constant. An ideal measure of $\frac{\Delta\alpha}{\alpha_\circ}$ would be obtained from ratios of lines that are spatially coincident with identical velocity structure. The multiple microwave transitions in the OH molecule may provide such an ideal diagnostic of the evolution of α provided that redshifts can be measured to at least one part in 10^5.

The OH molecule.—Each rotation state of the OH molecule is split by lambda-type doubling—the interaction of electronic angular momentum with the molecular rotation—and each of these states is further split by hyperfine splitting [5,6]. The net result is that each of the astronomically observed microwave transitions of OH is both a hyperfine transition and a transition between lambda-doubled levels. The two splittings depend differently on the fine structure constant α. Hyperfine transition frequencies in OH depend on terms of order $\mu_\circ \mu_I/(I\hbar a_\circ^3)$, where $\mu_\circ = e\hbar/2m_e c$ is the Bohr magneton, μ_I is the nuclear magnetic moment ($\mu_I \propto \mu_\circ$), I is the nuclear spin, and $a_\circ = \hbar^2/m_e e^2$ is the Bohr radius [5]. Hyperfine transition frequencies in OH thus follow the same α dependence as the HI 21 cm transition: $\nu_{\rm HF} \propto \alpha^4$.

The lambda doubling in OH depends on the molecular state. For the $^2\Pi_{3/2}$ state, which includes the OH ground state, the leading term in the lambda-doubling energy is independent of α: $B^3/(A\,E_{\Sigma-\Pi}) \propto \alpha^0$, where $B \propto \alpha^2$ is the rotational constant, $A \propto \alpha^4$ is the spin-orbit coupling constant (also called the fine structure interaction constant), and $E_{\Sigma-\Pi} \propto \alpha^2$ is the energy between the Σ and Π electronic states [5–8]. The A, B, and $E_{\Sigma-\Pi}$ terms also depend on the fundamental constants m_e, c, and $\hbar$. For the $^2\Pi_{1/2}$ state, the dominant term in the lambda-doubling energy does depend on α: $AB/E_{\Sigma-\Pi} \propto \alpha^4$ [7,8]. Second order corrections modify the α dependence of $A \propto \alpha^4$ at the 10%–25% level: $\nu_{3/2} \propto \alpha^{0.4}$ and $\nu_{1/2} \propto \alpha^{5.0}$. Higher order corrections modify the corrected exponent by $\lesssim 5\%$ [8–10], and these corrections are valid only for $\frac{\Delta\alpha}{\alpha_\circ} \ll 1$.

Hence, a generic $^2\Pi_{3/2}$ OH microwave transition (ignoring pure hyperfine transitions) can be written in terms of the fine structure constant as $\nu_{3/2} = \Lambda\alpha^{0.4} \pm (\Delta^+ \pm \Delta^-)\alpha^4$, where the choices of sign are independent (there are four possible lines), Λ sets the frequency of the lambda-doubled splitting, and $\Delta^\pm$ sets the strength of the hyperfine splitting for the $\pm$ parity lambda state. A generic $^2\Pi_{1/2}$ state can likewise be expressed as $\nu_{1/2} = \Lambda\alpha^5 \pm (\Delta^+ \pm \Delta^-)\alpha^4$, where the constants have different numerical values from the $^2\Pi_{3/2}$ case. Comparison of pairs of microwave transitions can thus determine the

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value of α in cosmic OH masers; one line fixes the velocity of the source, and the other determines α. The remarkable properties of the OH molecule provide a means to measure or constrain possible cosmic evolution of *α from a single species with built-in checks on systematic errors.* As illustrated in detail below, intercomparison of OH lines provides cases with no dependence on α which serve as benchmarks to quantify the systematics present in cases with a strong dependence on α. This property of the OH microwave transitions may provide the highly constrained method required to investigate claims of a time-varying fine structure constant.

OH ground state transitions.—The four 18 cm OH transitions in the ground $^2\Pi_{3/2}J = 3/2$ rotation state of OH are a combination of lambda-type doubling and hyperfine splitting [5] (Fig. 1). The dominant contribution comes from lambda doubling of order 1666 MHz, and each of these is doubled by hyperfine splitting of order 54 MHz. The hyperfine splitting is unequal between the upper and lower lambda-doubled states by 2 MHz, so that four 18 cm lines are possible in the ground rotation state of OH rather than two degenerate lines [10,11]:

$$\nu_{1612} = \Lambda\alpha^{0.4} - (\Delta^+ + \Delta^-)\alpha^4, \tag{1}$$

$$\nu_{1665} = \Lambda\alpha^{0.4} - (\Delta^+ - \Delta^-)\alpha^4, \tag{2}$$

$$\nu_{1667} = \Lambda\alpha^{0.4} + (\Delta^+ - \Delta^-)\alpha^4, \tag{3}$$

$$\nu_{1720} = \Lambda\alpha^{0.4} + (\Delta^+ + \Delta^-)\alpha^4, \tag{4}$$

where Λ sets the magnitude of the lambda doubling and Δ^+ and Δ^- set the magnitude of the hyperfine splitting of the upper and lower lambda-doubled states, respectively (Fig. 1). For $\alpha_\circ = 0.007\,297\,352\,533(27)$ (1998 CODATA recommended value), $\nu_{1665} = 1665.401\,84(10)$ MHz, and $\nu_{1667} = 1667.359\,03(10)$ MHz [12], we obtain $\Lambda = 11\,926.363\,09(51)$ MHz. For $\nu_{1720} = 1720.529\,98(10)$ MHz, we obtain $\Delta^+ = 9.720\,353(25) \times 10^9$ MHz, and $\Delta^- = 9.375\,256(25) \times 10^9$ MHz. These values for Λ and $\Delta^\pm$ determine a frequency for the final line of $\nu_{1612} = 1612.230\,89(12)$ MHz, which agrees with the measured value of 1612.231 01(20) MHz [12]. From $\alpha_\circ$ (α today) and the derived coefficients, we obtain the size of the lambda doubling and the hyperfine splitting: $\nu_\Lambda = \Lambda\alpha_\circ^{0.4} = 1666.380\,44(7)$ MHz, $2\Delta^+\alpha_\circ^4 = 55.128\,14(14)$ MHz, and $2\Delta^-\alpha_\circ^4 = 53.170\,95(14)$ MHz. Note that ν_Λ has a value equal to the mean of the 1667 and 1665 MHz lines and the mean of the 1720 and 1612 MHz lines; this is the closure criterion for the ground rotation state of OH.

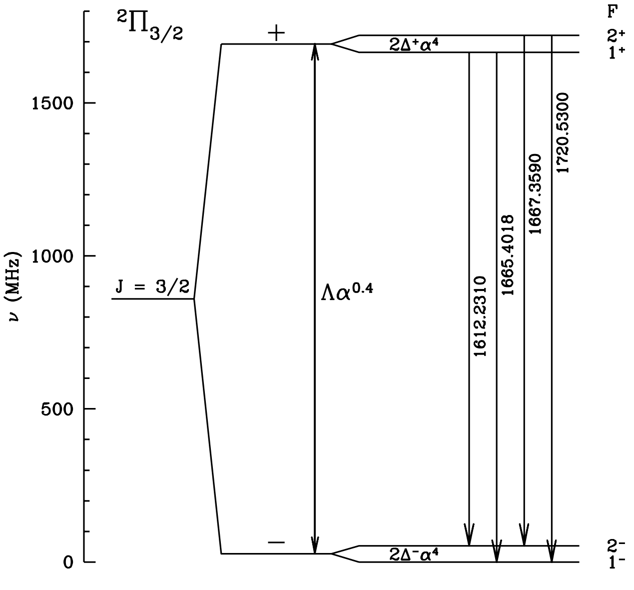

FIG. 1. The lambda doubling and hyperfine splitting of the $^2\Pi_{3/2}$ ground state of the OH molecule to scale. The 18 cm transitions are as labeled in MHz, and the parameters Λ and $\Delta^\pm$ are related to the size of the lambda doubling and hyperfine splitting, respectively. The zero point of the diagram is arbitrarily set to the lowest energy level.

The main lines observed in OH megamasers are at 1665 and 1667 MHz, with the latter dominant. We can form two quantities from the observed frequencies of these lines which isolate powers of α:

$$\Delta\nu \equiv \nu_{1667} - \nu_{1665} = 2(\Delta^+ - \Delta^-)\alpha^4, \tag{5}$$

$$\Sigma\nu \equiv \nu_{1667} + \nu_{1665} = 2\Lambda\alpha^{0.4} \tag{6}$$

such that the ratio $Y = \Delta\nu/\Sigma\nu = \alpha^{3.6}(\Delta^+ - \Delta^-)/\Lambda$. In terms of the fractional change in this ratio at a redshift z and the difference in redshift derived from the separation and average of the 1665 and 1667 MHz lines,

$$\frac{\Delta Y}{Y} \equiv \frac{Y_z - Y_\circ}{Y_\circ} = \frac{z_{\Sigma\nu} - z_{\Delta\nu}}{1 + z_{\Delta\nu}} = \frac{\alpha^{3.6} - \alpha_\circ^{3.6}}{\alpha_\circ^{3.6}} \simeq 3.6\frac{\Delta\alpha}{\alpha_\circ}, \tag{7}$$

where

$$\frac{\Delta\nu_\circ}{\Delta\nu_z} \equiv 1 + z_{\Delta\nu}, \qquad \frac{\Sigma\nu_\circ}{\Sigma\nu_z} \equiv 1 + z_{\Sigma\nu}, \tag{8}$$

$\Delta\alpha = \alpha - \alpha_\circ$, and $|\Delta\alpha| \ll \alpha_\circ$. The difference between the measured redshifts of the difference and sum of the main OH lines is thus of the same order of magnitude as the fractional change in the fine structure constant. Note that the change in $\Delta\nu$ expected for $\frac{\Delta\alpha}{\alpha_\circ} = 10^{-5}$ is of order 100 Hz, which is the accuracy to which the 18 cm OH line frequencies have been measured experimentally. Note, however, that a $\Delta\nu$ formed from the 1720 and 1612 MHz lines would have the same dependence on α but have substantially lower spectral resolution requirements than above (the change is of order 4 kHz, a factor of 55 larger). The OH satellite lines at 18 cm have been detected in only a few local starburst galaxies [13,14], so the prospects for detecting these lines at higher redshifts are poor. Detection of even a single satellite 18 cm line would provide a useful constraint on α (a factor of 27 better than is possible with $\Delta\nu$).

The evolution in the fine structure constant can be obtained from comparisons of any two OH lines if they originate from the same physical region. The most likely lines are the main 18 cm OH lines at 1667 and 1665 MHz:

$$\frac{z_{1665} - z_{1667}}{1 + z_{1667}} \simeq 1.8\left(\frac{\Delta\alpha}{\alpha_\circ}\right)\left(\frac{\Sigma\nu\Delta\nu}{\nu_{1667}\nu_{1665}}\right)_\circ. \tag{9}$$

The constant factor on the right-hand side of Eq. (9) refers to the rest frequencies of the OH lines and has a value of 0.002 35. This is a poor method for constraining fine structure constant evolution because it requires extremely precise redshift measurements. The comparison of the 1667 and 1665 MHz lines combine like powers of α, so the size of the effect reduces to the ratio between the difference in hyperfine splittings ($\Delta\nu \simeq 2$ MHz) and the line frequency. More sensitive measurements should use ratios of lines with different dependence on α such as the 5 cm transitions of OH. Regions with 5 or 6 cm OH transitions are likely to be physically conterminous with 18 cm and CO transition regions [15,16], especially in absorption systems.

6 cm transitions ($^2\Pi_{1/2}J = 1/2$).—The OH 6 cm transitions have been detected in absorption in five nearby OHMs, and the properties of the 18 and 6 cm lines appear to be correlated [15]. The three 6 cm $^2\Pi_{1/2}J = 1/2$ OH lines have frequencies 4660.242(3), 4750.656(3), and 4765.562(3) MHz [17]. These can be expressed in a similar manner to the 18 cm transitions:

$$\nu_{4660} = \Lambda_6\alpha^5 - (\Delta_6^- + \Delta_6^+)\alpha^4, \tag{10}$$

$$\nu_{4751} = \Lambda_6\alpha^5 + (\Delta_6^- - \Delta_6^+)\alpha^4, \tag{11}$$

$$\nu_{4766} = \Lambda_6\alpha^5 + (\Delta_6^- + \Delta_6^+)\alpha^4. \tag{12}$$

Note that the "+" and "−" states in $^2\Pi_{1/2}J = 1/2$ are reversed from the $^2\Pi_{3/2}J = 3/2$ ground state; the 4751 MHz line is the analog to the 1667 MHz line [11]. From the laboratory values for the line frequencies, we obtain values for the 6 cm coefficients: $\Lambda_6 = 2.277\,517\,8(10) \times 10^{14}$ MHz, $\Delta_6^- = 1.594\,21(7) \times 10^{10}$ MHz, and $\Delta_6^+ = 2.6283(7) \times 10^9$ MHz. Hence, the hyperfine splittings are quite unequal: $2\Delta_6^+\alpha_\circ^4 = 14.906(4)$ MHz and $2\Delta_6^-\alpha_\circ^4 = 90.414(4)$ MHz. Local thermodynamic equilibrium (LTE) ratios of the 4660, 4751, and 4766 MHz lines are 1:2:1 [18]. Observations of the nearest OHMs find that the absorption in these lines deviates somewhat from LTE, but the 4751 MHz line still tends to dominate [15].

Since the 6 cm lines are of nearly equal strength, it is likely that if any are detected, there will be at least two detectable lines [15]. Comparison of well-separated pairs of 6 cm lines produces $\frac{\Delta\alpha}{\alpha_\circ}$ "gain" factors of order $\Delta\nu_6/\nu \simeq 0.02$, where $\Delta\nu_6$ is the line separation. Comparing the dominant lines at 18 and 6 cm we obtain

$$\frac{z_{4751} - z_{1667}}{1 + z_{1667}} \simeq -\frac{\Delta\alpha}{\alpha_\circ}\left(1.8\frac{\Sigma\nu}{\nu_{1667}} + \frac{1}{2}\frac{\Sigma\nu_6}{\nu_{4751}}\right)_\circ, \tag{13}$$

where $\Sigma\nu_6 = 2\Lambda_6\alpha_\circ^5$ and the constant term is 4.59. This is a dramatic improvement over the 1665 to 1667 MHz line comparison (by a factor of nearly 2000), and for $\Delta\alpha/\alpha_\circ = 10^{-5}$, the resolution required for OH lines is 10's of kHz which is easily achieved. Equation (13) applies to the comparison of *any* 18 cm line to *any* 6 cm line, offering the possibility for multiple measurements of α from a single system. One can also obtain an accurate α-independent zero point by comparing $\Delta\nu$ to $\Delta\nu_6 = 2(\Delta_6^- + \Delta_6^+)\alpha^4$ to reveal any velocity offsets between 18 and 6 cm OH regions:

$$\frac{z_{\Delta\nu_6} - z_{\Delta\nu}}{1 + z_{\Delta\nu}} = 0. \tag{14}$$

Hence, comparison of 18 and 6 cm OH lines offers a sensitive method for detecting changes in α that includes redundant checks on statistical and systematic errors.

5 cm transitions ($^2\Pi_{3/2}J = 5/2$).—Absorption in a 5 cm OH line has been detected in just one OHM, Arp 220 [19]. The 5 cm OH lines have frequencies 6016.746(5), 6030.7485(2), 6035.0932(2), and 6049.084(8) MHz [17,18,20]. These can be expressed in a similar manner to the 18 cm transitions:

$$\nu_{6017} = \Lambda_5\alpha^{0.4} - (\Delta_5^- + \Delta_5^+)\alpha^4, \tag{15}$$

$$\nu_{6031} = \Lambda_5\alpha^{0.4} - (\Delta_5^- - \Delta_5^+)\alpha^4, \tag{16}$$

$$\nu_{6035} = \Lambda_5\alpha^{0.4} + (\Delta_5^- - \Delta_5^+)\alpha^4, \tag{17}$$

$$\nu_{6049} = \Lambda_5\alpha^{0.4} + (\Delta_5^- + \Delta_5^+)\alpha^4. \tag{18}$$

Note that the + and − states in $^2\Pi_{3/2}J = 5/2$ are reversed from the $^2\Pi_{3/2}J = 3/2$ ground state; the 6035 MHz line is the analog to the 1667 MHz line [11]. From the laboratory values for the first three line frequencies, we obtain values for the 5 cm coefficients: $\Lambda_5 = 431\,77.898(1)$ MHz, $\Delta_5^- = 3.2350(9) \times 10^9$ MHz, and $\Delta_5^+ = 2.4690(9) \times 10^9$ MHz. From these, we predict $\nu_{6049} = 6049.096(4)$ MHz, which is in fair agreement with the measured value. The hyperfine splittings in this case are only slightly unequal: $2\Delta_5^+\alpha_\circ^4 = 14.0025(50)$ MHz and $2\Delta_5^-\alpha_\circ^4 = 18.3472(50)$ MHz. LTE ratios of the 6017, 6031, 6035, and 6049 MHz lines are 1:14:20:1 [18].

Comparing the dominant lines at 18 and 5 cm we obtain

$$\frac{z_{6035} - z_{1667}}{1 + z_{1667}} \simeq 1.8\frac{\Delta\alpha}{\alpha_\circ}\left(-\frac{\Sigma\nu}{\nu_{1667}} + \frac{\Sigma\nu_5}{\nu_{6035}}\right)_\circ, \tag{19}$$

where $\Sigma\nu_5 = 2\Lambda_5\alpha^{0.4}$. The constant term is 0.000 45, which is smaller than the 1665 to 1667 MHz line comparison by a factor of 5. Comparing any 18 cm line to any 5 cm line gives the same order of magnitude α gain factor, to within a factor of 2. The difference in the hyperfine splitting between the lambda-doubled levels of $^2\Pi_{3/2}J = 5/2$ is so small that it provides poor leverage on α and requires extremely accurate redshift determinations. The hyperfine splitting of these levels is small overall, so detection of the satellite 5 cm lines would be of limited use (and unlikely).

OH vs HI.—The 21 cm hyperfine transition of HI is proportional to $\mu_p \mu_\circ/(\hbar a_\circ^3)$, where $\mu_p = g_p e\hbar/(4m_p c)$ and g_p is the proton g factor. In terms of α, the 21 cm line frequency is proportional to $\alpha^4(g_p m_e^2/m_p)$ modulo factors of $\hbar$ and c. The ratios of the 1667 or 1665 MHz lines or their sum to the 21 cm line can thus provide a measurement of α:

$$\frac{z_{\mathrm{HI}} - z_{1667}}{1 + z_{1667}} \simeq -1.8 \frac{\Delta\alpha}{\alpha_\circ} \left(\frac{\Sigma\nu}{\nu_{1667}}\right)_\circ \simeq -3.6 \frac{\Delta\alpha}{\alpha_\circ}. \qquad (20)$$

Comparison of the 1665 MHz line or $\Sigma\nu$ to HI produces the same relationship. For $\Delta\alpha/\alpha_\circ = 10^{-5}$, redshifts must be determined to about 4 parts in 10^5. This method does not require detection of the 1665 MHz line, but if it is detected, it provides a second determination of α. This is a promising avenue to measure $\alpha(z)$, with a check of systematics provided by the α-independent ratio $\Delta\nu/\nu_{\mathrm{HI}}$:

$$\frac{z_{\mathrm{HI}} - z_{\Delta\nu}}{1 + z_{\Delta\nu}} = 0. \qquad (21)$$

The $\Delta\nu/\nu_{\mathrm{HI}}$ ratio can provide an anchor for the method and indicate the influence of physical and/or velocity offsets between OH and HI, whereas the $\nu_{1667}/\nu_{\mathrm{HI}}$ ratio provides the maximum detectability of a change in α.

OH vs CO.—The rotational transitions of CO (and other diatomic molecules with balanced electronic angular momentum) have frequencies proportional to $\hbar/(Ma_\circ^2)$, where M is the reduced mass [6]. In terms of α, the rotational transitions of CO are proportional to $\alpha^2 m_e^2/M$ modulo factors of $\hbar$ and c. The ratio of the 1667 or 1665 MHz line to a CO rotational transition can thus provide a measurement of α:

$$\frac{z_{\mathrm{CO}} - z_{1667}}{1 + z_{1667}} \simeq -1.6 \frac{\Delta\alpha}{\alpha_\circ} \left(\frac{\nu_{1665}}{\nu_{1667}}\right)_\circ. \qquad (22)$$

For the 1665 MHz line, the constant term is inverted and differs from unity by about 0.1%. For $\frac{\Delta\alpha}{\alpha_\circ} = 10^{-5}$, redshifts must be determined to about 2 parts in 10^5. While comparisons of CO to OH transitions do not offer any α-independent line ratios, the sum and difference of 18 cm OH lines do offer some leverage on systematic errors:

$$\frac{z_{\mathrm{CO}} - z_{\Delta\nu}}{1 + z_{\Delta\nu}} \simeq 2 \frac{\Delta\alpha}{\alpha_\circ}; \qquad \frac{z_{\mathrm{CO}} - z_{\Sigma\nu}}{1 + z_{\Sigma\nu}} \simeq -1.6 \frac{\Delta\alpha}{\alpha_\circ}. \qquad (23)$$

Conclusions.—The remarkable properties of the microwave transitions in the OH molecule provide a robust method to measure deviations in α over cosmic time *from a single species.* This approach eliminates the largest systematic errors present in other determinations of α and provides estimates of the remaining statistical and systematic errors. The most promising method for measuring α is the comparison of 18 and 6 cm OH lines. This method includes α-independent line ratios which can identify the true size of statistical and systematic errors. Also promising are comparisons of OH lines to the HI 21 cm line and CO and other molecular rotation transitions, but only HI provides checks on systematics.

Deep surveys for OH megamasers (and OH gigamasers) are under way from the local Universe to $z \simeq 4$ and a subset of the new discoveries will have spectra appropriate for measurements of α. Several OH absorption systems have already been identified out to $z = 0.9$ [3] and more will be found in the near future. In the meantime, more precise laboratory measurements of the microwave transitions in OH would eliminate some of the uncertainty in the proposed techniques.

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