# Sensitivity of hyperfine structure to nuclear radius and quark mass variation

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To search for the temporal variation in the fundamental constants, one needs to know dependence of atomic transition frequencies on these constants. We study the dependence of the hyperfine structure of atomic *s* levels on nuclear radius and, via radius, on quark masses. An analytical formula has been derived and tested by the numerical relativistic Hartree-Fock calculations for Rb, $Cd^+$, Cs, $Yb^+$, and $Hg^+$. The results of this work allow the use of the results of past and future atomic clock experiments and quasar spectra measurements to put constraints on time variation in the quark masses.

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## I. INTRODUCTION

Interest in the variation in the fundamental constants is motivated by theories unifying gravity and other interactions. Indications that the fundamental constants might have varied slightly from those of the distant past have been found in Big Bang nucleosynthesis and quasar absorption spectra (see, e.g., reviews in [1–3]). Most publications report only constraints on possible variations in fundamental constants (see, e.g., reviews in [3–6]). Very stringent limits on the present time variation in the fundamental constants have been obtained in the atomic clock experiments (see, e.g., Refs. [7–19]). The majority of recent works have been devoted to the variation in the fine-structure constant $\alpha$. However, the hypothetical unification of all interactions implies that the variation in the dimensionless strong-interaction parameter $X_q=m_q/\Lambda_{QCD}$ [where $m_q=(m_u+m_d)/2$ is the average current-quark mass and $\Lambda_{QCD}$ is the quantum chromodynamics (QCD) scale] may be larger than the variation in $\alpha$ (see, for example, [20,21] and the references therein). In all intermediate calculations it is convenient to assume that the strong-interaction scale $\Lambda_{QCD}$ does not vary, so we will speak of the variation in masses. (This means that we measure masses in units of $\Lambda_{QCD}$.) We will restore the explicit appearance of $\Lambda_{QCD}$ in the final answers.

In a previous paper [22] calculations of the sensitivity of the nuclear radii to quark mass variation were performed. In the present Brief Report we calculate the dependence of hyperfine transition frequency on nuclear radius (a preliminary approximate analytical result of this work was presented in Ref. [22]). Combining the results of the present work and Ref. [22], we calculate the dependence of the hyperfine structure (hfs) on the quark masses and the dimensionless strong-interaction parameter $X_q=m_q/\Lambda_{QCD}$. These calculations are needed to use the results of very accurate atomic clock experiments to obtain constraints on the variation in the fundamental constants.

The result of the present work is presented as a simple analytical formula. To test this formula and improve the accuracy, we have performed numerical relativistic Hartree-Fock calculations for all atoms of experimental interest Rb, $Cd^+$, Cs, $Yb^+$, and $Hg^+$ (and Tl in excited $7s$ state). They happened to be atoms and ions with one *s*-wave electron above closed shells. One can use our analytical formula for other atoms where the hyperfine structure is dominated by *s*-wave electrons. For other electrons the effect of the nuclear radius variation is small and may be neglected.

## II. DEPENDENCE OF HYPERFINE TRANSITION FREQUENCY ON NUCLEAR RADIUS AND QUARK MASS

It was found in Ref. [22] that the variation in a nuclear radius $r_n$ can be related to variation in quark mass by

$$\frac{\delta r_n}{r_n} \approx 0.3\frac{\delta m_q}{m_q}. \tag{1}$$

Numerical factor of 0.3 in Eq. (1) is approximately the same for all nuclei. Then the variation in the frequency of a hyperfine transition $\omega_h$ may be presented as

$$\frac{\delta \omega_h}{\omega_h} \approx 0.3k_{hr}\frac{\delta m_q}{m_q}, \tag{2}$$

where

$$k_{hr}=\frac{\delta\omega_h/\omega_h}{\delta r_n/r_n}. \tag{3}$$

In this section we calculate $k_{hr}$ using analytical and numerical approaches.

To take into account finite nuclear size in the magnetic dipole hfs Hamiltonian, we approximate the nucleus by a uniformly magnetized sphere. Then the Hamiltonian has the form

$$\hat{H}_{hfs}=-\frac{e}{c}\boldsymbol{\mu}\cdot[\mathbf{n}\times\boldsymbol{\alpha}]U(r),$$

$$U(r)=\begin{cases}\dfrac{r}{r_n^3}, & r<r_n\\ \dfrac{1}{r^2}, & r\geq r_n.\end{cases} \tag{4}$$

Here $\mathbf{n}=\mathbf{r}/r$, $\boldsymbol{\alpha}$ is Dirac matrix, $\boldsymbol{\mu}$ is nuclear magnetic moment, and $r_n$ is nuclear radius.

For the analytical consideration we use a model of the nucleus where the nuclear charge is considered to be uni-

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TABLE I. The sensitivity of the hyperfine transition frequency to variation in the nuclear radius, analytical ($k_{hr}$) from Eqs. (7) and (11), and numerical ($k_{hr\text{-}cal}$) results.

| | Atom or ion | | | | | | |
|---|---|---|---|---|---|---|---|
| | $^{87}_{37}$Rb | $^{111}_{48}$Cd$^+$ | $^{133}_{55}$Cs | $^{171}_{70}$Yb$^+$ | $^{199}_{80}$Hg$^+$ | $^{205}_{81}$Tl($7s$) | $^{233}_{87}$Fr |
| $k_{hr}$ | −0.010 | −0.017 | −0.024 | −0.048 | −0.077 | −0.081 | −0.111 |
| $k_{hr\text{-}cal}$ | −0.0096 | −0.0171 | −0.0242 | −0.0492 | −0.0778 | −0.0798 | −0.1082 |
| $C$ | 1.9514 | 2.0034 | 2.0338 | 2.0500 | 2.0050 | 1.9623 | 1.9563 |

formly distributed about a sphere of radius $r_n$. Such a charge distribution corresponds to the potential

$$V(r) = \begin{cases} -\dfrac{Ze^2}{r_n}\left(\dfrac{3}{2} - \dfrac{r^2}{2r_n^2}\right), & r < r_n \\ -\dfrac{Ze^2}{r}, & r \geq r_n. \end{cases} \tag{5}$$

It is convenient to present the hyperfine frequency as $\omega_h = \omega_0(1-\delta_h)$, where $\omega_0$ is the frequency at $r_n=0$ and $\delta_h$ describes the change in the hfs frequency due to finite nuclear radius $r_n$. For potential (5) the electron wave functions in the vicinity of the nucleus can be found analytically and we obtain the following approximate expression for $\delta_h$ (see the Appendix for details):

$$\delta_h \approx \frac{72}{35}\left(\frac{Zr_n}{a_B}\right)^{2\gamma-1}, \tag{6}$$

where $\gamma = \sqrt{1-Z^2\alpha^2}$ and $a_B$ is the Bohr radius. Then we obtain

$$k_{hr} = \frac{\delta\omega_h/\omega_h}{\delta r_n/r_n} = -\frac{(2\gamma-1)\delta_h}{1-\delta_h}. \tag{7}$$

To check these results with a more accurate approach, we calculate atomic hfs constants using the relativistic Hartree-Fock method (see, e.g., [23]). Relativistic Hartree-Fock Hamiltonian for atoms with one external electron above closed shells can be written as

$$\hat{H}^{HF} = c\boldsymbol{\alpha}\cdot\mathbf{p} + (\beta-1)mc^2 + V_{nuc}(r) + V^{N-1}. \tag{8}$$

Here $V_{nuc}(r)$ is nuclear potential and $V^{N-1}$ is the self-consistent Hartree-Fock potential of the closed-shell atomic core containing $N-1$ atomic electrons. Nuclear potential $V_{nuc}(r)$ is found by numerical integration of the Fermi-type distribution of the nuclear charge. We assume the same electric and magnetic radius. The same Hamiltonian (8) is used for core and valence states. The hfs frequencies are expressed via expectation values of hfs Hamiltonian (4) over wave functions of the valence electron calculated with Hamiltonian (8). Note that neither core polarization nor correlation effects are important for the *relative* change in the hfs frequency for $s$-wave energy levels since the polarization and correlation corrections are dominated by the matrix elements of the hyperfine interaction between the $s$-wave orbitals. (The hyperfine matrix elements between the $p,d,\ldots$ orbitals are significantly smaller.) We have tested this conclusion using the full-scale many-body calculations for the Cs hyperfine structure using approach developed in our previous work [24]. With the accuracy of ~1% the polarization and correlation corrections do not change the relative value of the effect of the variation. (To avoid misunderstanding we should note that the polarization and correlation corrections change the hyperfine-structure constant by ~40%.)

To find the change in the hyperfine frequency due to the change in nuclear radius, we perform calculations for at least two different nuclear radii and then calculate the following derivative numerically:

$$\frac{\delta\omega_h}{\delta r_n} = \frac{\omega_h(r_n+\delta r_n) - \omega_h(r_n-\delta r_n)}{2\delta r_n}. \tag{9}$$

The values of $k_{hr\text{-}cal}$ found from the Hartree-Fock calculations are presented in Table I. Using Eq. (7) we can express $\delta_h$ in a form similar to Eq. (6),

$$\delta_h \approx C(Zr_n/a_B)^{2\gamma-1}, \tag{10}$$

where $C$ is a fitting factor found from a comparison of the results of calculations with formula (10). The values of $C$ for some atoms are presented in Table I. Its variation from atom to atom is small and its average value is 1.995. Using $r_n = 1.1A^{1/3}$ fm and the total number of nucleons $A \approx 2.5Z$ leads to the formula

$$\delta_h = 1.995 \times (2.8\times 10^{-5}Z^{4/3})^{2\gamma-1}, \tag{11}$$

which can be used for any medium or heavy atom. Note that this result agrees with the purely analytical result [Eq. (6)] to the accuracy of few percent.

Now we can use expression (2) to calculate the sensitivity of $\omega_h$ to the quark mass due to the variation in nuclear radius (parameter: $k_{hq}=0.3k_{hr}$). All results are displayed in Table II.

TABLE II. The sensitivity of the hyperfine structure to variation in $\alpha$ (parameter $K_{rel}$) and to the quark mass to strong-interaction scale ratio $m_q/\Lambda_{QCD}$ (parameter $k=k_\mu+k_{hq}$).

| | Atom or ion | | | | |
|---|---|---|---|---|---|
| | $^{87}_{37}$Rb | $^{111}_{48}$Cd$^+$ | $^{133}_{55}$Cs | $^{171}_{70}$Yb$^+$ | $^{199}_{80}$Hg$^+$ |
| $K_{rel}$ | 0.34 | 0.6 | 0.83 | 1.5 | 2.28 |
| $k_\mu$ | −0.016 | 0.125 | 0.009 | −0.085 | −0.088 |
| $k_{hq}$ | −0.003 | −0.005 | −0.007 | −0.014 | −0.023 |
| $k$ | −0.019 | 0.120 | 0.002 | −0.099 | −0.111 |

Also presented in Table II are the parameters $K_{rel}$, $k_\mu$, and $k=k_\mu+k_{hq}$. $K_{rel}$ is the sensitivity of the hyperfine structure to variation in $\alpha$ derived from the results of the atomic many-body calculations [25]. Parameter $k_\mu$ is the sensitivity of the nuclear magnetic moment to quark mass calculated in Ref. [26].

It is convenient to present the final results using the ratio of the hyperfine energy $E_h=\hbar\omega_h$ to the atomic unit of energy $E_a=m_e e^4/\hbar^2$. Atomic experiments always measure the ratio of two atomic frequencies. The atomic unit of energy $E_a$ cancels out in such ratios. Following Ref. [26] we define the parameter $V$ through the relation

$$\frac{\delta V}{V}=\frac{\delta(E_h/E_a)}{E_h/E_a}. \tag{12}$$

Then one can use Table II to find the dependence of the hyperfine transition frequencies on the variation in the fundamental constants using the following formula from Ref. [26]:

$$V=\alpha^{2+K_{rel}}\left(\frac{m_q}{\Lambda_{QCD}}\right)^k\frac{m_e}{m_p}. \tag{13}$$

A number of limits on variation in $V$ from different experiments are presented in Ref [26]. These results give the best present time limits on the variation in $m_q/\Lambda_{QCD}$. For example, for $\omega_h(^{87}\mathrm{Rb})/\omega_h(^{133}\mathrm{Cs})$, we have

$$X(\mathrm{Rb/Cs})=\frac{V(^{87}\mathrm{Rb})}{V(^{133}\mathrm{Cs})}=\alpha^{-0.49}\left(\frac{m_q}{\Lambda_{QCD}}\right)^{-0.021}, \tag{14}$$

and the result of measurements in [9] can be presented as a limit on the variation in $X$:

$$\frac{1}{X(\mathrm{Rb/Cs})}\frac{dX(\mathrm{Rb/Cs})}{dt}=(-0.5\pm5.3)\times10^{-16}/\mathrm{yr}. \tag{15}$$

Using a very stringent limit on the variation in $\alpha$ obtained using our calculations [25,27] and measurements in Ref. [19],

$$\frac{1}{\alpha}\frac{d\alpha}{dt}=(-1.6\pm2.3)\times10^{-17}/\mathrm{yr}, \tag{16}$$

we may find the variation in $X_q=m_q/\Lambda_{QCD}$ from Eqs. (14) and (15):

$$\frac{1}{X_q}\frac{dX_q}{dt}=(0.3\pm2.5)\times10^{-14}/\mathrm{yr}. \tag{17}$$

Note that the effect of the variation may be enhanced by 2–3 orders of magnitude in a number of molecules where the hyperfine splitting is approximately equal to an interval between the rotational levels [28].

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## APPENDIX

The analytical approach presented here is very similar to those used in Ref. [29]. To simplify all expressions we use atomic units $\hbar=e=m_e=1$ and $c=1/\alpha$ in this appendix.

We use an electron wave function in the form

$$\psi_\kappa^{m_j}(\mathbf{r})=\frac{1}{r}\begin{pmatrix} f_\kappa(r)\chi_\kappa^{m_j}(\hat{\mathbf{r}}) \\ ig_\kappa(r)\chi_{-\kappa}^{m_j}(\hat{\mathbf{r}})\end{pmatrix}, \tag{A1}$$

where $\chi_\kappa^{m_j}$ are spherical spinors. For an $s$-orbital the initial terms of a power-series solution of the radial wave functions inside the nucleus are

$$f_n=ax\left[1-\left(\frac{3}{8}\frac{Z^2}{c^2}+\frac{1}{2}Zr_n\right)x^2+\cdots\right], \tag{A2}$$

$$g_n=-\frac{aZ}{2c}x^2\left[1-\left(\frac{1}{5}+\frac{9}{40}\frac{Z^2}{c^2}+\frac{3}{10}Zr_n\right)x^2+\cdots\right], \tag{A3}$$

where $x=r/r_n$. Only those terms explicit in Eqs. (A2) and (A3) will be retained for further calculation. The external radial wave functions take the form of Bessel functions

$$f_e=(\gamma+\kappa)[J_{2\gamma}(y)+bY_{2\gamma}(y)]-\frac{y}{2}[J_{2\gamma-1}(y)+bY_{2\gamma-1}(y)], \tag{A4}$$

$$g_e=\frac{Z}{c}[J_{2\gamma}(y)+bY_{2\gamma}(y)], \tag{A5}$$

where $\kappa=(-1)^{j-l+1/2}(j+1/2)$,

$$\gamma=\sqrt{\kappa^2-\alpha^2Z^2},\quad y=\sqrt{8Zr}. \tag{A6}$$

As the binding energy of the electron is small in comparison to the potential energy, it has been neglected in the calculation of Eqs. (A2)–(A5). The constants $a$ and $b$ are found such that the wave functions remain continuous at $r=r_n$. For small $r_n$ they may be approximated by

$$a=\frac{(2Zr_n)^\gamma}{\Gamma(2\gamma)}\left(-\frac{1}{5}(2\gamma+3)+\frac{3}{80}\frac{Z^2}{c^2}(3\gamma+7)+\frac{1}{20}Zr_n(3\gamma+7)\right)^{-1}, \tag{A7}$$

$$b=-\frac{a\pi(2Zr_n)^\gamma}{\Gamma(1+2\gamma)}\left(-\frac{1}{5}(2\gamma-3)+\frac{3}{80}\frac{Z^2}{c^2}(3\gamma-7)+\frac{1}{20}Zr_n(3\gamma-7)\right). \tag{A8}$$

As we shall only consider relative changes in the hyperfine interaction, normalization of the wave functions is not necessary. The first-order correction to the energy is simply the $s$-wave expectation value of the hyperfine interaction, which may be shown to be

$$\omega_h = \langle s|\hat{H}_{hfs}|s\rangle = k\int U(r) f g dr, \tag{A9}$$

where $k$ is a constant [30]. In the limit of zero nuclear radius this becomes

$$\omega_0 = k\int_0^\infty \frac{1}{r^2} f_0 g_0 dr = \frac{kZ^2(1-2\kappa)}{c(\gamma-4\gamma^3)}, \tag{A10}$$

where $f_0=f_e$ and $g_0=g_e(r_n=0)$. We define a relative change in the hyperfine interaction $\delta_h$ by $\omega_h=\omega_0(1-\delta_h)$,

$$\delta_h = -\frac{k}{\omega_0}\int_0^{r_n}\left(\frac{r}{r_n^3} f_n g_n - \frac{1}{r^2} f_0 g_0\right) dr - \frac{k}{\omega_0}\int_{r_n}^\infty \frac{1}{r^2}(f_0\delta g_e + g_0 \delta f_e) dr, \tag{A11}$$

where $\delta g=g_e-g_0$ and $\delta f=f_e-f_0$. For small $r_n$ these integrals result in

$$\delta_h = -\frac{a^2\gamma(4\gamma^2-1)}{Zr_n}\left(\frac{1}{35} - \frac{13}{1008}\frac{Z^2}{c^2} - \frac{13}{756}Zr_n + \frac{1}{640}\frac{Z^4}{c^4} + \frac{1}{240}\frac{Z^3 r_n}{c^2} + \frac{1}{360}Z^2 r_n^2\right) + \frac{(2Zr_n)^{2\gamma-1}2\gamma(1+\gamma)(1+2\gamma)}{3\Gamma(1+2\gamma)^2} + \frac{b(4\gamma^2-1)}{3\pi Zr_n}. \tag{A12}$$

Keeping only leading in $Zr_n$ terms reduces this to

$$\delta_h \approx \tfrac{72}{35}(Zr_n)^{2\gamma-1}. \tag{A13}$$

Differentiation of $\omega_h$ with respect to $r_n$ and rearranging yields

$$\frac{\delta\omega_h}{\omega_h} = -\frac{(2\gamma-1)\delta_h}{1-\delta_h}\frac{\delta r_n}{r_n}. \tag{A14}$$


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