Magic Frequencies for Cesium Primary-Frequency Standard

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We consider microwave hyperfine transitions in the ground state of cesium and rubidium atoms which are presently used as the primary and the secondary frequency standards. The atoms are confined in an optical lattice generated by a circularly polarized laser field. We demonstrate that applying an external magnetic field with appropriately chosen direction may cancel dynamic Stark frequency shift making the frequency of the clock transition insensitive to the strengths of both the laser and the magnetic fields. This can be attained for practically any laser frequency which is sufficiently distant from a resonance.

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The microwave transition between Cs hyperfine levels is used to define the second, the unit of time. The best accuracy of the Cs standard is now achieved in a fountain clock [1,2]. For optical clocks with neutral atoms the best results are obtained using optical lattices where atoms are trapped in minima (or maxima) of a laser standing wave [3–7]. Here a laser producing an optical lattice operates at a "magic frequency" where the light shift of the clock transition is zero (due to cancellation of the light shifts of the lower and upper clock levels). To extend this successful technique to microwave frequencies one must firstly check if the magic frequencies exist for such transitions. In our recent work [8] we found the magic frequencies for aluminum and gallium hyperfine transitions where the valence electron is in the $p_{1/2}$ state (the magic frequency there is a result of mixing of the $p_{1/2}$ and $p_{3/2}$ states by the hyperfine interaction-see details in [8]). However, we have not found any magic frequencies for Cs, Rb and other atoms with the $s_{1/2}$ electron in the ground state. In Ref. [8], we considered the case of the linear polarization of the lattice laser light. In the present Letter we show that the cancellation of the light shifts for Cs, Rb and other atoms with $s_{1/2}$ (or $p_{1/2}$) electron exist if (1) the laser light in optical lattice has a circular (or elliptical) polarization, and (2) the angle θ between the quantizing magnetic field B and the light wave vector k is close to 90°.

By varying θ one can achieve the cancellation of the light shifts for any frequency ω , i.e., any frequency can be "magic". Numerical calculation of $\theta(\omega)$ has been performed for the cesium and rubidium microwave frequency standards.

Hyperfine clock transitions in magnetic field.—Let us start from the case of no magnetic field. The light shift of an individual atomic energy level in a circularly polarized laser field is given by (see, e.g., [9])

$$\delta E_{nFM_F}^{\text{circ}} = -\left(\frac{1}{2}\mathcal{E}\right)^2 \left[\alpha_{nF}^s(\omega) + A\alpha_{nF}^a(\omega)\frac{M_F}{2F} - \alpha_{nF}^T(\omega)\frac{3M_F^2 - F(F+1)}{2F(2F-1)}\right].$$
 (1)

Here \mathcal{E} is the amplitude of the laser field, $\mathbf{F} = \mathbf{I} + \mathbf{J}$; *I* is the nuclear spin; *J* is the total electron momentum; M_F is projection of \mathbf{F} on the quantization axis; α^s , α^a and α^T are the scalar, vector (axial) and tensor polarizabilities of an atom. The quantization axis here is along the propagation of the laser light and *A* is the degree of the circular polarization (A = 1 for the right-hand and A = -1 for the left-hand polarizations).

In the presence of a sufficiently large magnetic field the direction of the quantization axis is along the magnetic field. In this case the shift depends on the angle θ between the magnetic field **B** and the direction of light propagation determined by the wave vector **k**. This gives an additional factor $\cos\theta$ in the vector polarizability contribution [the central term in (1)]. The tensor contribution [the last term in (1)] is multiplied by a factor $\xi(\theta, \phi)$ which depends on orientations of the *B* field and polarization; for the circular polarization $\xi(\theta) = (3\cos^2\theta - 1)/2$.

$$\delta E_{nFM_F}^{\text{circ}} = -\left(\frac{1}{2}\mathcal{E}\right)^2 \left[\alpha_{nF}^s(\omega) + (\cos\theta)A\alpha_{nF}^a(\omega)\frac{M_F}{2F} - \xi(\theta,\phi)\alpha_{nF}^T(\omega)\frac{3M_F^2 - F(F+1)}{2F(2F-1)}\right].$$
 (2)

The effect of the laser field on the frequency of a microwave clock transition can be found by using (2) for both levels and taking the difference. We are interested in cases when this difference is zero, so that the frequency is insensitive to the laser field.

The relevant clock shift of a transition between hyperfine levels arises in the second (quadratic in laser field) and the third order of perturbation theory (quadratic in laser field + linear in hyperfine interaction). In the case of Al and Ga hyperfine-structure (hfs) transitions in the $p_{1/2}$ ground states considered in Ref. [8], the zero frequency shift is due to cancellation between scalar and tensor hfsinduced polarizabilities. Clock states with $M_F = 0$ were considered so that the vector part did not contribute. The tensor polarizabilities of atoms in the p states are strongly enhanced due to small value of the fine structure interval between the $p_{1/2}$ and $p_{3/2}$ states which goes to the energy denominator of the tensor polarizability (produced by the mixing of $p_{1/2}$ and $p_{3/2}$ states by the hyperfine interaction). There is no such enhancement for cesium and other microwave frequency standards based on atoms with the $s_{1/2}$ ground state. As a consequence, there are no magic frequencies if the vector term plays no role. This was discussed in Ref. [8].

Note, however, that the contributions of the scalar and tensor polarizabilities to the frequency shifts in the $s_{1/2}$ and $p_{1/2}$ hyperfine transitions are proportional to the hyperfine interaction and appear in the third order of the perturbation theory while the vector polarizability contribution exists even without the hyperfine interaction, so it appears in the lower (second) order of the perturbation theory. This means that for $A \cos \theta \sim 1$ the vector contribution is orders of magnitude larger. Therefore, by varying angle θ (or degree of the circular polarization A) we can always find some small value of the factor $A \cos \theta$ in the vector contributions and make the total light shift of the hyperfine frequency zero. (The second-order scalar light shift is identical for both clock levels and does not contribute to the clock shift.)

Consider, for example, a transition between hfs components which have different total angular momenta F and the same projection M_F . As seen from (2), the frequency shift for such a transition can be turned to zero practically for any frequency of laser field by controlling the orientation of the external magnetic field. This magic direction is given by

$$\cos\theta(\omega) = -\frac{2}{AM_F} \frac{\alpha_{F_2}^s(\omega) - \alpha_{F_1}^s(\omega)}{\alpha_{F_2}^a(\omega)/F_2 - \alpha_{F_1}^a(\omega)/F_1}.$$
 (3)

Here we neglect the tensor term which is small for cesium. The numerator of (3) is due to the third-order (second in the laser field and first in the hfs) scalar polarizabilities. Second-order polarizabilities (without the hfs) do not contribute to the energy difference because they do not depend on *F*. By contrast, the denominator is strongly dominated by the second-order vector polarizabilities. The formulas for second and third-order polarizabilities can be found below and in Refs. [9–11].

Because of the extra hfs operator in the numerator of (3) $\cos(\theta)$ is small which means that the magnetic field is directed almost perpendicular to the propagation of the laser light. Figure 1 shows the results of calculations for

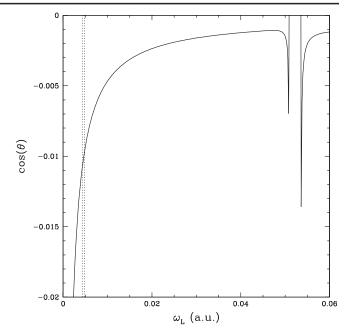


FIG. 1. Calculated $\cos(\theta)$ for ¹³³Cs, where θ is the angle between magnetic field and the light propagation which makes the laser frequency to be *magic*. Vertical lines correspond to frequencies of the CW CO₂ laser.

the clock transition in cesium between hfs states of $F_1 = 3$ and $F_2 = 4$ with $M_F = 3$ in both cases. The results for $\cos(\theta)$ show complicated behavior in the vicinity of the $6s \cdot np_{1/2}$ and $6s \cdot np_{3/2}$ resonances. The first two $6s \cdot 6p_{1/2}$ and $6s-6p_{3/2}$ resonances are included in Fig. 1. For all frequencies sufficiently distant from resonances $\cos(\theta)$ is a smooth function of the frequency of laser field. The angle θ which makes the frequency to be *magic* is always close to 90°. As $\omega \to 0$, $\cos\theta(\omega) \propto 1/\omega$, and the angle changes rapidly at small frequencies which may be advantageous. Indeed, the rapid change of θ means that the magic frequency is less sensitive to uncertainties in θ . Two close dotted vertical lines on Fig. 1 show frequencies of the CO₂ laser ($\omega_L = 0.43$ a.u. and $\omega_L = 0.48$ a.u.) which fell into this region. Corresponding values of θ are $\theta = 90.62^{\circ}$ and $\theta = 90.55^{\circ}$.

Figure 2 shows the results of similar calculations for the F = 1, $M_F = 1$ to F = 2, $M_F = 1$ hfs transition in the ground $5s_{1/2}$ state of ⁸⁷Rb. All notations are the same as for Fig. 1. Magic angles for the frequencies of the CO₂ laser are $\theta = 91.77^{\circ}$ and $\theta = 91.57^{\circ}$.

As usual, the linear Zeeman shift may be eliminated if we average the frequencies of the hyperfine transitions with the opposite sign of M_F , for example $M_F = 3$ and $M_F = -3$. However, to keep the cancellation of light shifts in place, we must have the same value of the products $AM_F \cos\theta$ in both transitions. This may be achieved by the simultaneous change of signs of M_F and circular polarization A.

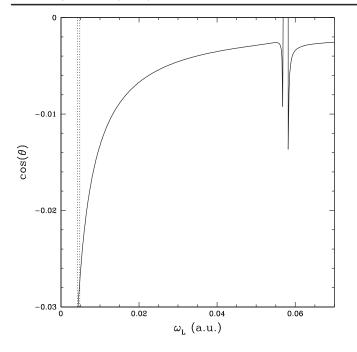


FIG. 2. Calculated $\cos(\theta)$ for ⁸⁷Rb.

Another solution for eliminating the linear Zeeman shift is employing the hyperfine components with $M_{F_1} = -M_{F_2}$. The equation for the magic angle would be similar to Eq. (3), except the difference of the vector polarizabilities in the denominator would be replaced by their sum.

A more accurate treatment of the effects of the B field requires simultaneous consideration of the magnetic interaction and vector light shift. The latter is equivalent to a "pseudomagnetic" field directed along the light wave vector **k**. The effective Hamiltonian may be presented in the following form:

$$H = -\frac{\mathbf{F} \cdot \mathbf{Q}}{F},\tag{4}$$

where

$$\mathbf{Q} = \boldsymbol{\mu}_F \mathbf{B} + V \mathbf{n}_k,$$

and

$$V = \left(\frac{1}{2}\mathcal{E}\right)^2 A \alpha^a_{nF}(\omega) \frac{1}{2}.$$

Here $\mathbf{n}_k = \mathbf{k}/k$ is the unit vector along \mathbf{k} and μ_F is the magnetic moment of the hyperfine component *F*. The energy levels of this Hamiltonian are given by

$$E = -\frac{M_F Q}{F},\tag{5}$$

where

$$Q = \sqrt{(\mu_F B)^2 + 2V\mu_F B\cos\theta + V^2}$$

$$\approx \mu_F B + V\cos\theta + \frac{V^2}{(2\mu_F B)} + \cdots.$$

A new feature here is the quadratic vector term which should be subtracted from the result of measurements to find an accurate value of the hyperfine transition frequency.

Note that in an optical lattice one actually has a standing wave. In this case it is appropriate to talk about the direction of the photon spin $\mathbf{S}_{ph} = A\mathbf{n}_k$ (or the direction of rotation of the light electric field) instead of the direction of the wave vector $\mathbf{n}_k = \mathbf{k}/k$. Indeed, to have the needed standing wave, in the reflected wave both \mathbf{n}_k and A change sign while $\mathbf{S}_{ph} = A\mathbf{n}_k$ and the direction of the light electric field are the same.

Calculation of polarizabilities.—The second-order dynamic vector polarizability is given by

$$\begin{aligned} \alpha^{a}_{n(IJ)F}(\omega) &= -\sqrt{\frac{24F(2F+1)}{(F+1)}} \begin{cases} J & F & I \\ F & J & 1 \end{cases} \\ &\times \omega \sum_{n'J'} (-1)^{J'+I+F} \begin{cases} 1 & 1 & 1 \\ J & J & J' \end{cases} \\ &\times \frac{|\langle nJ||D||n'J'\rangle|^{2}}{(E_{nI} - E_{n'J'})^{2} - \omega^{2}}. \end{aligned}$$

The third-order AC Stark shift (involving two light fields and hfs) is given by the frequency-dependent generalization of the DC Stark shift presented previously in Refs. [10-12] in the context of the black-body radiation clock shift. The structure of the resulting expressions is presented in Ref. [8]. Explicit formulas are lengthy and will be presented elsewhere.

To perform the calculations we follow the procedure described in detail in our previous work [11]. We use ab initio relativistic Hartree-Fock method in the frozencore approximation to construct an effective singleelectron Hamiltonian \hat{H}_0 . Then an all-order correlation potential $\hat{\Sigma}^{(\infty)}$ [13] is used to build a complete set of single-electron basis states. These states are the eigenstates of the $\hat{H}_0 + \hat{\Sigma}^{(\infty)}$ Hamiltonian and are usually referred to as the Brueckner orbitals. Because of the $\hat{\Sigma}^{(\infty)}$ operator they include the dominant polarization interaction between core and valence electrons. This approach gives fraction of a per cent accuracy for the energies of valence states. To calculate matrix elements of the electric dipole and hyperfine interactions we also include the effect of core polarization by external field. This is done by means of the timedependent Hartree-Fock method [14], which is equivalent to the well-known random-phase approximation. The resulting accuracy for the polarizabilities is about 1% (see Ref. [11] for detailed discussion).

Conclusion.—We conclude that microwave clocks (Cs, Rb, ...) using specially engineered magic optical lattices may be an interesting alternative to the fountain clocks. We have shown that, in principle, the light shift and the linear Zeeman shift may be eliminated. The atoms in the lattice are confined to a tiny volume. This may help in solving such problems as a homogeneity of magnetic field and

cooling the chamber to reduce the thermal black-body radiation shift. However, the expected accuracy of the optical-lattice microwave clocks is yet to be explored. This problem deserves further theoretical and experimental investigation. Even if the precision of such clocks turns out be less competitive than that of the fountains, the microwave lattice clocks have a clear advantage of a smaller apparatus size. This may be important for many applications, e.g., for the spacecraft applications including navigation systems and precision tests of fundamental symmetries in space.

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