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Possibility of an optical clock using the $6\,^1S_0 \rightarrow 6\,^3P_0^o$ transition in ^{171,173}Yb atoms held in an optical lattice

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We report calculations assessing the ultimate precision of an atomic clock based on the 578 nm $6\,^1S_0 \rightarrow 6\,^3P_0$ transition in Yb atoms confined in an optical lattice trap. We find that this transition has a natural linewidth less than 10 mHz in the odd Yb isotopes, caused by hyperfine coupling. The shift in this transition due to the trapping light acting through the lowest order ac polarizability is found to become zero at the *magic* trap wavelength of about 752 nm. The effects of Rayleigh scattering, multipole polarizabilities, vector polarizability, and hyperfine induced electronic magnetic moments can all be held below 1 mHz (about one part in 10^{18}). In the case of the hyperpolarizability, however, larger shifts due to nearly resonant terms cannot be ruled out without an accurate measurement of the magic wavelength.

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Optical atomic clocks offer opportunities for creating improved time standards as well as for looking for changes in fundamental constants over time, measuring gravitational redshifts, and timing pulsars. Compared with microwave atomic clocks, optical clocks have the intrinsic advantage that optical transitions have a much higher frequency and potentially much higher line Q than microwave transitions. Moreover, optical frequency comb techniques [1] now permit different optical frequencies to be compared with each other at the 10^{-17} level or better and to be linked to microwave clocks as well. Optical transitions in alkaline earth atoms offer remarkable possibilities for clocks. In addition to the relatively sharp $^1S_0 \rightarrow {}^3P_1^o$ intercombination line already in use [2], there occurs the much sharper $^1S_0 \rightarrow {}^3P_0^o$ line in odd isotopes. This one-photon transition is forbidden in even isotopes, but in odd isotopes acquires a weak $E1$ amplitude induced by the internal hyperfine coupling of the nuclear spin. Doppler and recoil shifts can be virtually eliminated by confining very cold atoms in an optical lattice trap. The lattice will be ''Stark-free'' (i.e., the ground and excited states undergo the same light shift) at a certain *magic* frequency of the laser beam. At this frequency the clock transition is unshifted and relatively insensitive to the laser polarization.

Katori [3] has pointed out these advantages for ^{87}Sr, and the $5\,^1S_0 \rightarrow 5\,^3P_0^o$ transition in this isotope has recently been observed [4]. Also, Sr atoms have been held in an optical lattice at the laser wavelength appropriate for a Stark-free $5\,^1S_0 \rightarrow 5\,^3P_1^o$ transition, and this transition has been observed free of Doppler and recoil shifts [5]. The magic frequency for the Sr clock was evaluated recently in Ref. [6] and measured in Ref. [7]. In Ref. [6] an estimate of systematic uncertainties for Sr was also carried out.

Ytterbium has two stable odd isotopes ^{171}Yb and ^{173}Yb, which also appear to be excellent candidates for an atomic standard, using the $6\,^1S_0 \rightarrow 6\,^3P_0^o$ transition at the convenient wavelength 578 nm [8]. The atoms are readily trapped into a magneto-optical trap (MOT) operating on either the strong $6\,^1S_0 \rightarrow 6\,^1P_1^o$ line or the $6\,^1S_0 \rightarrow 6\,^3P_1^o$ intercombination line, and in the latter case have been cooled to microkelvin temperatures by Sisyphus cooling [9]. These isotopes have also been successfully confined in an optical dipole trap [10]. The bosonic isotopes have recently been Bose-Einstein-condensed [11]. In this paper we present a calculation of the natural linewidth of the clock transition, which turns out to be less than 10 mHz, and also a calculation of the Stark-free wavelength of an optical lattice trap for the clock transition. This wavelength turns out to be about 752 nm, reachable with adequate power by a tunable Ti:sapphire laser. We also estimate the size of the polarizability due to higher magnetic dipole and electric quadrupole optical moments. In addition, we estimate the Rayleigh and Raman scattering rates in the optical lattice, which can limit the coherence lifetime of the clock transition. Finally, we compute the small but important hyperfine-induced Zeeman shift in the excited state and the vector light shift, which can cause a small Stark-shift dependence on the polarization of the trapping light.

Our results indicate that a light intensity of 10 kW/cm^2 would create a convenient trap depth of 15 μK at the magic wavelength, while perturbations to the clock frequency could be held below the millihertz level (10^{-18} relative shift)—with one possible exception. Larger shifts due to accidental near resonances in the hyperpolarizability cannot be ruled out without an accurate measurement of the magic wavelength. For a thorough discussion of other potential sources of error in atomic clocks, e.g., the second-order Doppler shift, blackbody radiation, etc., see Ref [12].

All the calculations reported in this paper were carried out using the relativistic many-body code described in Refs.

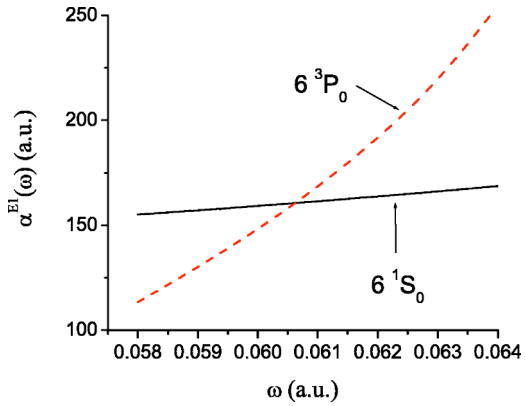

FIG. 1. Electric dipole ac polarizabilities for $6\,^1S_0$ (solid line) and $6\,^3P_0$ (dashed line) states of Yb. The polarizabilities are shown as a function of laser frequency ω.

[13–15]. The formalism employed is a combination of the configuration-interaction (CI) method in the valence space with many-body perturbation theory (MBPT) for core-polarization effects. The effective core-polarization (self-energy) operator is adjusted so that the experimental energy levels are well reproduced. In addition, the dressing of the external electromagnetic field (so-called core shielding) is included in the framework of the random-phase approximation. In the following we refer to this many-body method as CI+MBPT. For Yb, the CI+MBPT method has an accuracy of a few percent for electric dipole matrix elements and magnetic dipole hyperfine constants [16,17]. Unless specified otherwise, we use atomic units ($|e|=\hbar=m_e\equiv 1$) throughout the paper.

In the proposed design, the Yb atoms are confined to sites of an optical lattice (formed by a standing-wave laser field of frequency ω and amplitude of electric field $\mathcal{E}_0$). To the leading order in intensity and the fine-structure constant, the laser field shifts the clock transition frequency ω_0 by

$$\delta\omega_0(\omega)=-\{\alpha^{E1}_{6\,^3P^o_0}(\omega)-\alpha^{E1}_{6\,^1S_0}(\omega)\}(\mathcal{E}_0/2)^2, \qquad (1)$$

where $\alpha^{E1}_X(\omega)$ is the ac electric dipole polarizability of level X,

$$\alpha^{E1}_X(\omega)=2\sum_Y \frac{E_Y-E_X}{(E_Y-E_X)^2-\omega^2}|\langle X|D_z|Y\rangle|^2. \qquad (2)$$

We carried out calculations of the $E1$ ac polarizability using the CI+MBPT method. We summed over the intermediate states in Eq. (2) using the Dalgarno-Lewis-Sternheimer method [18]. The results of the calculations for both $6\,^1S_0$ and $6\,^3P^o_0$ states are shown in Fig. 1. The two dynamic polarizabilities intersect at $\omega^*=0.0606$ a.u. At this "magic" frequency the lowest-order differential light shift, Eq. (1), vanishes. It is worth noting that at ω^* the sum (2) for the ground state is dominated by the $6s6p\,^1P^o_1$ state and for the $6\,^3P^o_0$ level by the $6s7s\,^3S_1$ state. We estimate that the calculated scalar ac polarizabilities are accurate to a few percent.

In general, for a linear laser polarization the second-order light shift of level X can be represented as a sum over 2^J-pole polarizabilities $\alpha^{(J\lambda)}_X$ (λ distinguishes between electric, $\lambda=1$, and magnetic, $\lambda=0$, multipoles):

$$\delta E_X=-\frac{\mathcal{E}_0^2}{4}\sum_{J\lambda}\alpha^{(J\lambda)}_X(\omega). \qquad (3)$$

The contribution to the light shift due to the circular polarization and hyperpolarizability will be addressed below. When the total angular momentum of the level X is equal to zero these ac polarizabilities are expressed as

$$\alpha^{(J\lambda)}_X(\omega)=\frac{J+1}{J}\frac{2J+1}{[(2J+1)!!]^2}(\alpha\omega)^{2J-2}\times\sum_Y\left\{\frac{(E_Y-E_X)|\langle Y||Q^{(J\lambda)}||X\rangle|^2}{(E_Y-E_X)^2-\omega^2}\right\},$$

with $Q^{(J\lambda)}$ being the relevant multipole operators [19]. Typically, the $E1$ polarizability (2) overwhelms this sum. Compared to the $E1$ contribution, the higher-order multipole polarizabilities are suppressed by a factor of $(\alpha\omega)^{2J-2}$ for EJ and by a factor of $\alpha^2(\alpha\omega)^{2J-2}$ for MJ multipoles. We verified that at the magic frequency there are no resonant contributions for the next-order $E2$ and $M1$ polarizabilities, and we expect $\alpha^{(E2,M1)}\lesssim 10^{-6}\alpha^{(E1)}$, similar to the case of Sr [6]. At the same time, we notice that a core-excited state $4f^{13}(^2F^o_{7/2})5d_{5/2}6s^2\ J=5$ may become resonant with an excitation from the $6\,^3P^o_0$ level. The relevant $M5$ polarizability is highly suppressed, and we anticipate that the magic frequency will be only slightly shifted by the presence of this state.

Higher-order corrections to the differential frequency shift Eq. (1) arise due to terms quartic in the field strength $\mathcal{E}_0$. This fourth-order contribution is expressed in terms of ac hyperpolarizability $\gamma(\omega)$. The expression for $\gamma(\omega)$ [20] has a complicated energy denominator structure exhibiting both single- and two-photon resonances. While for the ground state there are no such resonances, for $6\,^3P^o_0$ a two-photon resonance may occur for $6s8p\,^1P^o_1$ and $6s8p\,^3P^o_J$ intermediate states. Due to theoretical errors in calculations of the magic frequency we cannot reliably predict if the two-photon resonances would occur. Since the resonance contributions may dominate $\gamma(\omega)$, we cannot provide a reliable estimate of the fourth-order frequency shift. The estimate may be carried out as soon as the magic frequency is measured with sufficient resolution. The required accuracy of the measurements would depend on how close the magic frequency is to the position of the two-photon resonance. As a possible indication of the effect on the clock frequency, we notice that for Sr [6] the resulting correction to the energy levels was a few millihertz at a trapping laser intensity of 10 kW/cm^2. This systematic uncertainty can be controlled by studying the dependence of the level shift on the laser intensity [5].

The $6\,^3P^o_0$ state decays due to an admixture from $J=1$ states caused by the hyperfine interaction. In this paper we

restrict our attention to the hyperfine structure (hfs) due to the nuclear magnetic moment μ. We write this interaction as $H_{\rm hfs}=(\mu/\mu_N\cdot\mathcal{T}_e^{(1)})$, where the tensor $\mathcal{T}_e^{(1)}$ acts on the electronic coordinates and μ_N is the nuclear magneton. We employ the following nuclear parameters: for ^{171}Yb, the nuclear spin $I=1/2$ and magnetic moment $\mu=0.4919\mu_N$, and for ^{173}Yb, $I=5/2$ and $\mu=-0.6776\mu_N$. Using first-order perturbation theory, the hfs-induced transition rate is given by

$$A_{\rm hfs}(6\,^3P_0^o)=\frac{4\alpha^3}{27}\frac{(I+1)}{I}(\mu/\mu_N)^2\omega_0^3|S|^2, \tag{4}$$

where the sum S is defined as

$$S=\sum_{\gamma'}\frac{\langle 6^1S_0||D||\gamma'\rangle\langle\gamma'||\mathcal{T}_e^{(1)}||6\,^3P_0^o\rangle}{E(\gamma')-E(6\,^3P_0^o)} \tag{5}$$

and $\omega_0=E(6\,^3P_0^o)-E(6\,^1S_0)$.

To estimate the rate we restricted the summation over intermediate states to the nearest-energy $6\,^1P_1^o$ and $6\,^3P_1^o$ states. Using the CI+MBPT method we computed hfs couplings, $\langle 6\,^3P_0^o||\mathcal{T}_e^{(1)}||6\,^3P_1^o\rangle=-6685$ MHz and $\langle 6\,^3P_0^o||\mathcal{T}^{(1)}||6\,^1P_1^o\rangle=4019$ MHz and inferred the values of hfs-induced dipole matrix elements from lifetime measurements [21,22]. The resulting hfs-induced lifetimes of the $6\,^3P_0^o$ level are 20 and 23 s for ^{171}Yb and ^{173}Yb isotopes, respectively. Since we truncated the summation over intermediate states, we anticipate that the resulting accuracy of these lifetimes is on the order of 10%.

Coherence of atomic states may be lost due to scattering of laser photons (Rayleigh and Raman processes [23]). These are second-order processes. In particular, the Rayleigh (heating) rate for both the $6\,^3P_0^o$ and ground states may be expressed in terms of the ac polarizability:

$$\gamma_h=\alpha^4\frac{32\pi}{3}(\omega^*)^3[\alpha^{E1}(\omega^*)]^2I_L,$$

where I_L is the intensity of laser (we took into account that the maximum intensity in an optical lattice is four times larger than I_L.) At the magic frequency ω^* the values of the ac polarizability for both states are equal to 160 a.u. (see Fig. 1). For a laser intensity of 10 kW/cm^2, the resulting rate is on the order of 10^{-2} s^{-1}. As to the Raman rates, there are no Raman transitions originating from the ground state. The final states for transitions from the $6^3P_0^o$ are the $J=1,2$ sublevels of the same $6\,^3P_J^o$ fine-structure multiplet. We estimate this rate by approximating the relevant second-order sum with the dominant contribution from the $6s7s\,^3S_1$ intermediate state. The resulting Raman scattering rate is also on the order of 10^{-2} s^{-1} for 10 kW/cm^2 laser.

The total magnetic moment of the Yb atom is composed of the nuclear and electronic magnetic moments. Disregarding shielding of externally applied magnetic fields by atomic electrons, the g factor due to the nuclear moment is given by $\delta g_{\rm nuc}=-(1/m_p)(\mu/\mu_N)/I$, where m_p is the proton mass. The numerical values of $\delta g_{\rm nuc}$ are -5.4×10^{-4} for ^{171}Yb and 1.48×10^{-4} for ^{173}Yb. The electronic magnetic moment of the $6\,^3P_0^o$ state arises due to mixing of levels caused by the hyperfine interaction, i.e., the same mechanism that causes the $6\,^3P_0^o$ state to decay radiatively. This correction may be expressed as

$$\delta g_{\rm hfs}\approx\frac{\sqrt{8}}{3}\frac{1}{I}\frac{\mu}{\mu_N}\frac{\langle 6\,^3P_1^o||\mathcal{T}_e^{(1)}||6\,^3P_0^o\rangle}{E(6\,^3P_1^o)-E(6\,^3P_0^o)}.$$

The computed values of the $\delta g_{\rm hfs}$ correction are 2.9×10^{-4} for ^{171}Yb and -8.1×10^{-5} for ^{173}Yb, which imply that millihertz shifts would be produced by microgauss magnetic fields. Fields can readily be calibrated and stabilized to this level using magnetic shielding.

The hyperfine interaction also induces residual vector (axial) $\alpha_{\gamma F}^A(\omega)$ and tensor $\alpha_{\gamma F}^T(\omega)$ ac polarizabilities. For $J=0$ levels there is no tensor contribution for the ^{171}Yb isotope ($I=1/2$), and it can be shown that for ^{173}Yb ($I=5/2$) it vanishes when the hfs interaction is restricted to the dominant magnetic dipole term. For a nonzero degree of circular polarization $\mathcal{A}$, the relevant correction to the light shift of level γF is

$$\delta E_{\gamma F}^{(A)}=-\frac{M}{2F}\mathcal{A}\alpha_{\gamma F}^A(\omega)\left(\frac{1}{2}\mathcal{E}_0\right)^2, \tag{6}$$

where, for $J=0$, $F=I$ and M is the magnetic quantum number. Using third-order perturbation theory and the formalism of quasienergy states [20], we arrived at an expression for $\alpha_{\gamma F}^A(\omega)$ which contains two dipole and one hyperfine operators in various orderings and double summations over intermediate states. Analyzing these expressions, we find that the vector polarizability of the $6\,^3P_0^o$ state is much larger than that for the ground state, as in the case of Sr [6]. For Sr, Katori *et al.* [6] estimated the vector polarizability by adding a hfs correction to the energy levels of intermediate states in Eq. (2). Our analysis is more complete, and we find that the dominant effect is not due to corrections to the energy levels but rather to perturbation of the $6\,^3P_0$ state by the hfs operator. The resulting values of $\alpha_{6\,^3P_0}^A(\omega^*)$ are -0.10 a.u. for ^{171}Yb and 0.075 a.u. for ^{173}Yb. Using these values in the above equation, we find that holding $\mathcal{A}$ to $<10^{-6}$ with fields of 10 kW/cm^2 would keep shifts in the clock frequency below the millihertz level. This requirement on optical polarization is not an extreme one, and in the special case of a one-dimensional 1D optical lattice could be relaxed significantly by orienting the quantization axis (defined by the external magnetic field) perpendicular to the trap axis.

In conclusion, we have analyzed the possibility of creating a highly precise optical clock operating on the $6\,^1S_0\rightarrow6\,^3P_0^o$ transition in odd isotopes of atomic Yb. According to our calculations, the natural linewidth is about 10 mHz, and the magic wavelength for producing zero Stark shift of this transition in an optical lattice trap is about 752 nm. We have examined possible sources of shifts and broadening due

to both the optical trapping fields and any magnetic fields, and find they should not perturb the clock above the 10^{-18} level, except for possible larger near-resonant terms in the hyperpolarizability. An accurate measurement of the magic wavelength will be needed to settle this last question.

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