Additional clock transitions in neutral ytterbium bring new possibilities for testing physics beyond the Standard Model

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We study the prospects of using transitions from the ytterbium ground state to metastable states at $E = 19710.388$ cm^{-1} and $E = 23188.518$ cm^{-1} as clock transitions in an optical lattice clock. Having more than one clock transition in Yb could benefit the search for new physics beyond the Standard Model via studying the non-linearity of King's plot or the time-variation of the ratio of the frequencies of two clock transitions. We calculate the lifetime of the states, relevant transition amplitudes, systematic shifts, and the sensitivity of the clock transitions to a variation of the fine structure constant. We find that both clock transitions can probably support very high precision, similar to what is already achieved for the ^{1}S$_0$ - ^{3}P$^o_0$ clock transition.

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I. INTRODUCTION.

The search for new physics beyond the Standard Model (SM) with low-energy experiments requires extremely accurate measurements. The highest fractional accuracy has been achieved for atomic optical clocks such as based on Sr, Yb, Al$^+$, Hg, Hg$^+$, and Yb$^+$. It is now at the low-10^{-18} level [1–7]. When clock transitions are also sensitive to new physics beyond the SM, the benefit of using atomic clocks is enormous. At least two clock transitions must be available in order to produce a test of the SM. The clock transitions must have different sensitivity to new physics to avoid cancellation of the effect in the ratio of frequencies. A good example of such a system is the Yb$^+$ ion. It has two clock transitions, one is an electric quadrupole (E2) transition between the ground [Xe]$4f^{14}6s\ ^2$S$_{1/2}$ and the excited [Xe]$4f^{14}5d\ ^2$D$_{3/2}$ states, another is an electric octupole (E3) transition between the ground and the excited [Xe]$4f^{13}6s^2\ ^2$F$_{7/2}$ states. This second transition has high sensitivity to a variation of the fine structure constant [8] and to local Lorentz invariance violation [9], while the first transition can serve as an anchor.

It has been recently suggested that the search for a possible non-linearity of King's plot can be used in the search for new physics beyond the SM [10]. On a King's plot the ratios of isotope shifts for two atomic transition frequencies are plotted for several isotopes. In the absence of new physics all points are expected to be approximately on the same line (up to some small corrections [11]). Electron-nucleus interaction due to exchange of a hypothetical scalar particle produces a non-linearity of King's plot.

The minimum data needed to search for non-linearity of King's plot requires two transitions and four isotopes (leading to three isotope shifts against a reference isotope). The expected smallness of the effect suggests the use of clock transitions. The ytterbium atom has seven stable isotopes, one well-studied clock transition, and several metastable states which can probably be used in additional clock transitions. In this paper we study the [Xe]$4f^{14}6s6p\ ^3$P$^o_2$ and [Xe]$4f^{13}5d6s^2\ (7/2, 3/2)_2$ states. The numbers in parentheses are the angular momenta of the f-shell hole and of the d-electron. The subscript denotes the total electronic angular momentum $J = 2$.

II. CALCULATIONS AND ANALYSIS.

We perform atomic structure calculations with the CIPT method [12], which combines configuration interaction (CI) with the perturbation theory (PT). This allows to treat ytterbium atom as a system with sixteen external electrons so that states with excitations from the $4f$ subshell can be considered. We use random phase approximation (RPA) to calculate transition amplitudes. See Appendix for the details of the calculations.

The results for the energies of relevant low-energy states of Yb are presented in Table I. Note some small differences in the results compared to previous calculations [12]. This is due to differences in the basis and the size the effective CI matrix. These differences are within the accuracy of the method.

The calculated amplitudes and corresponding transition rates are presented in Table II. Using data from the Table we find that the lifetimes of the new clock states (number 4 and 5 in Table I) are about 15 s and 200 s respectively. This leads to the quality factors $Q = 2\pi\omega/R \approx 10^{16}$ and 10^{17}. The decay of these states is dominated by the M1 transitions to the ^{3}P$^o_1$ state. The rates for the M2 transitions between these clock states and the ground state are 2.5×10^{-4} s^{-1} and 1.5×10^{-5} s^{-1}, respectively. They are smaller than the rate of the hyperfine interaction-induced transition between ground and clock state number two (^{3}P$^o_0$) which varies between 10^{-2} and 10^{-1} s^{-1} depending on the isotope and the hyperfine structure components [16]. For comparison, they are larger than the rate of the hyperfine interaction-induced E3 transition in Yb$^+$ ions, which is $\sim 10^{-6}$ s^{-1} [17].

TABLE I: Energies and lifetimes of low-lying states of Yb. New clock states are shown in bold.

	State			Energy [cm^{-1}]		Lifetime
N			J	Expt. [14]	CIPT	
1	$4f^{14}6s^2$	^{1}S	0	0	0	∞
2[a]	$4f^{14}6s6p$	^{3}P^o	0	17288	17265	23-26[b] s
3	$4f^{14}6s6p$	^{3}P^o	1	17992	18327	500 ns
4	$\mathbf{4f^{14}6s6p}$	$\mathbf{^3P^o}$	**2**	**19710**	**19895**	**15[c] s**
5	$\mathbf{4f^{13}5d6s^2}$	**(7/2,3/2)^o**	**2**	**23188**	**24831**	**200[c] s**
6	$4f^{13}5d6s^2$	(7/2,3/2)^o	3	27445	27185	
7	$4f^{14}5d6s$	^{3}D	1	24489	27584	
8	$4f^{14}5d6s$	^{3}D	2	24751	27678	
9	$4f^{14}5d6s$	^{3}D	3	25271	27763	
10	$4f^{14}6s6p$	^{1}P^o	1	25068	24753	5 ns
11	$4f^{14}5d6s$	^{1}D	2	27677	28156	
12	$4f^{13}5d6s^2$	(7/2,5/2)^o	1	28857	29610	8 ns

[a] Current clock state.
[b] 23.0 s for ^{171}Yb and 26.0 s for ^{173}Yb [16].
[c] For even isotopes.

TABLE II: Transition amplitudes (A, in atomic units), corresponding rates (R) of spontaneous emission and experimental transition frequencies between some states of Table I. Numbers in square brackets indicate powers of ten. New clock transitions are shown in bold. To obtain $A_{\rm E2}$, $A_{\rm M2}$ in SI units, multiply by $e\,a_0^2$.

Transition	Type	A	ω [cm^{-1}]	R [s^{-1}]
3 - 1	E1	0.711	17992	2.0[+6]
10 - 1	E1	4.14	25068	1.8[+8]
12 - 1	E1	2.71	28857	1.2[+8]
4 - 1	**M2**	**0.61[-1]**	**19710**	**2.5[-4]**
4 - 3	M1	0.57[-2]	1718	6.7[-2]
4 - 5	M1	0.37[-4]	3478	
5 - 1	**M2**	**0.993[-2]**	**23188**	**1.5[-5]**
5 - 2	E2	1.43	5900	3.3[-4]
5 - 3	M1	0.277[-3]	5196	4.7[-3]
5 - 4	M1	0.170[-2]	3478	2.6[-5]
5 - 6	M1	0.25[-2]	4257	
5 - 12	M1	0.49[-2]	5669	
7 - 5	E1	0.531[-1]	1301	
8 - 5	E1	0.186	1563	
9 - 5	E1	0.453	2086	
11 - 5	E1	0.744[-1]	4489	

A. Rabi oscillations.

In this paper we focus on even Yb isotopes to avoid large Zeeman shifts in M2 clock transitions (see below). In even isotopes the ^{1}S$_0$ - ^{3}P$^o_0$ clock transition is extremely weak but can be opened by a magnetic field. We have computed the E1 amplitude (see Appendix) and find good agreement with the result of Ref. [18].

The Rabi frequency of a M2 transition is given by $\Omega_{\rm R} = E_0\,\alpha\,\omega\,A_{M2}$, (all values are in atomic units). Using the values of the M2 transition amplitudes from Table II we find $\Omega_R/2\pi = (44,\,8.5)\ {\rm Hz}\sqrt{I}/\sqrt{{\rm mW/cm^2}}$ for the 1 - 4 and 1 - 5 clock transition, respectively. The laser intensity I_π required to achieve a desired excitation time $T_\pi = \pi/\Omega_R \simeq 1\,$s is of order μW/cm^2 and lower, a very small value.

TABLE III: Dynamic polarizabilities of states 1 (third column) and 4 (fourth and fifth columns)(in a.u.). The magic wavelength is in bold.

ω (cm^{-1})	λ (nm)	$\alpha_{0,1}(\omega)$	$\alpha_{0,4}(\omega)$	$\alpha_{2,4}(\omega)$
0		142	425	-67
9060	**1104**	169	89	-80
17288	578	303	155	83
19710	507	311	655	32
23168	432	784	-76	199

B. Polarizabilities, magic frequency, black-body radiation and Stark shifts.

The shifts of the clock frequency due to the effect of black-body radiation (BBR), of the lattice laser field that traps the atoms, and of the clock laser field depend on the dipole polarizabilities of the clock states. For the ground and the ^{3}P$^o_0$ states they are well-known (see, e.g. [15, 19]). Therefore, we need to calculate the polarizabilities of the new clock states, 4 and 5. Details of the calculations for the state 4 can be found in the Appendix. The result for states 1 and 4 are shown in Table III.

For the BBR shift it is sufficient to consider the difference in polarizabilities $\Delta\alpha(0)$ of the two clock states at zero frequency. For the 1 - 4 clock transition, we use $\alpha_0(0) = 425$ a.u. for state 4, which leads to a $\Delta\alpha(0)$ approximately 1.6 times larger compared to the 1 - 2 clock transition [15, 19]. Correspondingly, the BBR shift is also 1.6 times larger, i.e. $\Delta\omega_{{\rm BBR},1-4} \simeq$ 1.6 Hz at 300 K [15].

The situation is more complicated for the $4f^{13}5d6s^2(7/2,3/2)^o_2$ state (number 5). As explained above, it cannot be treated as a two-valence-electron state and the method of Ref. [15] to calculate the polarizability is not applicable. On the other hand, we can use the results of Ref. [20] which demonstrated that the polarizabilities of atoms with open $4f$ shell are mostly determined by the $6s - np$ matrix elements and the $4f$-$5d$ excitation changes the polarizability insignificantly. Comparing energy intervals between the ground $4f^{14}6s^2$ and excited $4f^{14}6s6p$ configurations with the intervals between the $4f^{13}5d6s^2$ and $4f^{13}5d6s6p$ configurations, we conclude that the polarizability of state 5 might be 1.5 times larger than the polarizability of the ground state and it is unlikely to be larger that the polarizability of the clock state 2. This in turn means that the effect of BBR on the frequency of the clock transition 1 - 5 is smaller than $\Delta\omega_{{\rm BBR},1-2}$.

We may thus expect that for both new clock transitions the BBR shifts can be controlled, respectively, at the same level as or better than that for the current Yb clock

transition 1×10^{-18} [21].

The magic frequency ω_M for the lattice laser is found from $\Delta\alpha(\omega_M) = 0$. For the 1 - 4 transition it depends on J_z due to the contribution of the tensor polarizability $\alpha_2(\omega)$ of state 4. For $J = 2$ and $J_z = 0$ the total polarizability is $\alpha(\omega) = \alpha_0(\omega) - \alpha_2(\omega)$ (see Appendix). We find the longest magic wavelength to be $\omega_M = 1104\,\mathrm{nm}$ (Table III) It is sufficiently far from resonances and is experimentally easily realizable.

Finally, we estimate the clock transition Stark shift due to the clock laser electric field ("probe shift"). It is given by (in atomic units)

$$\Delta\omega_\mathrm{p} = -\frac{1}{2}\Delta\alpha(\omega)E_0^2. \tag{1}$$

Using the numbers from Table III and from Ref. [15] we find the frequency shift coefficients for the 1 - 2 and 1 - 4 transitions to be 15 and $16\,\mathrm{mHz}/(\mathrm{mW/cm^2})$, respectively. The first number is in exact agreement with the result of Ref. [18].

As was discussed above, the method of Ref. [15] is not applicable to state number 5. However, comparing energies and E1 transition amplitudes for states 4 and 5 (see Tables I and II), we conclude that the shift coefficient for the 1 - 5 transition is of the same order of magnitude as for the 1 - 4 transition.

These coefficients lead to negligible shifts, considering the required intensities I_π.

C. Electric quadrupole and Zeeman shifts.

The clock states considered in this work have the relatively large value of the total electronic angular momentum $J = 2$. This means that they will be sensitive to any external magnetic field and gradients of any electric field. We will consider the ways of dealing with these effects in even isotopes, which all have zero nuclear spin. The first-order Zeeman shift can be suppressed by considering transitions between states with $F_z = J_z = 0$ or by averaging over states with $\pm J_z$. For the present goals, the first approach appears more suitable.

The energy shift due to a gradient of a residual static electric field ε is described by a corresponding term in the Hamiltonian

$$\hat{H}_Q = -\frac{1}{2}\hat{Q}\frac{\partial\varepsilon_z}{\partial z}, \tag{2}$$

where $\hat{Q}$ is the atomic quadrupole moment operator ($\hat{Q} = |e|r^2Y_{2m}$, the same as for E2 transitions). The energy shift of a state with total angular momentum J is proportional of the atomic quadrupole moment of this state. It is defined as twice the expectation value of the $\hat{Q}$ operator in the stretched state

$$Q_J = 2\langle J, J_z = J|\hat{Q}|J, J_z = J\rangle. \tag{3}$$

Calculations similar to those described above give the values $Q_J = -18$ a.u. for state 4, and $Q_J = -5.3$ a.u. for state 5. For a state with projection J_z of the total angular momentum J, the shift is proportional to $3J_z^2 - J(J+1)$. Note that for $J = 2$ the shift has the same value but opposite sign for $J_z = 0$ and $J_z = \pm 2$. Therefore, averaging over these states can, at least in principle, suppress both electric quadrupole and linear Zeeman shifts. Alternatively, it is possible to reduce the quadrupole shift by measuring the transition frequency three times, with the magnetic field direction applied in three mutually orthogonal directions [22]. In this case one can use only states with $J_z = 0$ avoiding the linear Zeeman shift.

The quadratic Zeeman shift can be estimated using second-order perturbation theory,

$$\delta E_Z(J, J_z) = \sum_n \frac{|\langle n, J_n, J_z|\mu_z H_z|J, J_z\rangle|^2}{E_J - E_n}, \tag{4}$$

where $J_n = J, J \pm 1$ and summation goes over complete set of states. In most of cases summation in (4) is strongly dominated by terms within the same fine structure multiplet. This is because of small energy denominator and large value of magnetic dipole matrix elements. However, for clock state number 5 (see Table I) three states give significant contribution, states number 6, 10 and 12. The first two are within the same fine structure multiplet as clock state 5, while state 12 is strongly mixed with state 10. The Zeeman shifts calculated for the three clock states are presented in Table IV. There are several things to note:

(1) The largest shift coefficient is for the $^3\mathrm{P}_0^\mathrm{o}$ state. This is due to the small fine structure interval of 704 cm^{-1} between the $^3\mathrm{P}_0^\mathrm{o}$ and $^3\mathrm{P}_1^\mathrm{o}$ states.

(2) For state 4 the shift is extremely small for $J_z = \pm 2$ because there is no mixing with this state within the fine-structure multiplet. The shift is due to M1 matrix elements with states of different configurations. Such matrix elements are very small due to the orthogonality of the wave functions. The shift is further suppressed by large energy denominators.

(3) For state number 5 the shift coefficient for $J_z = \pm 2$ is also small. This is convenient since such states are also good for suppressing linear Zeeman shift and electric quadrupole shift (see above).

The quadratic Zeeman shift for the ground state is small, since there are no fine-structure contributions. I.e., it is much smaller than for the upper clock states and can be neglected in the difference. Altogether, the quadratic Zeeman shifts of the transition frequencies are sufficiently small to be compatible with a 10^{-18}-level clock inaccuracy.

D. Search for variation of the fine structure constant.

To search for a possible time variation of the fine structure constant α one needs to monitor a ratio of two clock frequencies over a long period of time. Atomic calculations are needed to link a variation of frequencies to a

TABLE IV: Second-order Zeeman shift coefficient for clock states in units $\mathrm{Hz/G^2}$. Numeration of the states is taken from Table I.

State	J	J_n	J_z	Shift		
				This work	Other	
2	0	1	0	-6.0[-2]	-6.2[-2][a]	-7(1)[-2][b]
4	2	1,2,3	0	1.2[-2]		
			1	9.2[-3]		
			2	-4.7[-7]		
5	2	1,2,3	0	-4.3[-3]		
			1	-3.4[-3]		
			2	-3.4[-3]		

[a]Theoretical estimation, Ref. [18].
[b]Experiment, Ref. [23].

TABLE V: Sensitivity of Yb clock transitions to variation of the fine structure constant.

Clock transition	Transition frequency ω [$\mathrm{cm^{-1}}$]	q [$\mathrm{cm^{-1}}$]	$K = 2q/\omega$
1 - 2	17288.439	2714[a]	0.31
1 - 4	19710.388	5505	0.56
1 - 5	23188.518	-44290	-3.82

[a]Ref. [24].

variation of α. It is convenient to express the atomic transition frequencies in a form $\omega = \omega_0 + q[(\alpha/\alpha_0)^2 - 1]$, where ω_0 and α_0 are present-time values of the frequency and and the fine structure constant, and q is the sensitivity coefficient which comes from calculations. Then

$$\frac{\partial}{\partial t} \ln \frac{\omega_1}{\omega_2} = \frac{\dot{\omega}_1}{\omega_1} - \frac{\dot{\omega}_2}{\omega_2} = \left(\frac{2q_1}{\omega_1} - \frac{2q_2}{\omega_2} \right) \frac{\dot{\alpha}}{\alpha}. \qquad (5)$$

To find the values of q for each transition we calculate the frequencies of the transitions at different values of α and then calculate the derivative numerically. The values of q and corresponding enhancement factors $K = 2q/\omega$ are presented in Table V. We see that the 1 - 5 transition is the most sensitive to the variation of the fine structure constant. If we compare it to the currently used 1 - 2 transition then

$$\frac{\dot{\omega}_1}{\omega_1} - \frac{\dot{\omega}_2}{\omega_2} = 4.12 \frac{\dot{\alpha}}{\alpha}. \qquad (6)$$

In other words, there is significant enhancement of the variation of the frequency ratio compared to the variation of the fine structure constant. The enhancement comes from the different nature of the two clock transitions. The clock transition 1 - 2 corresponds to the $s-p$ single-electron transition, while the clock transition 1 - 5 is the $f-d$ transition.

The current best laboratory limit on the present-day time variation of α stands at about 10^{-17} per year [25–27]. If the fractional uncertainty of both clock transitions can reduced to the 10^{-18} level (which is already the case for the 1 - 2 transition) then there are good prospects of further improvements of the limits of the time variation on the fine structure constant.

E. Search for new physics using the non-linearity of King's plot.

In the King's plot the isotope shift of an atomic transition is plotted against the isotope shift of another transition. This is done for several isotopes with every new isotope adding a new point on the plot. Normally, all points are on the same line. This is a consequence of the factorisation of the nuclear and electron variables in the field (volume) shift term. See Ref. [28] for the case of Yb. However, if there is a new interaction between atomic electrons and nucleus which depends on the number of neutrons, the factorisation and thus linearity might be broken. The minimum set of data to study the non-linearity of King's plot requires two transitions and four isotopes (leading to three isotope shifts against a reference isotope). The expected small value of the effect demands for the high accuracy of the measurements. Therefore, it is best to use clock transitions.

The ytterbium atom has seven stable isotopes, two of them have non-zero nuclear spin. The choice of isotope depends on whether the hyperfine interaction is needed to induce the transition. This is an issue for the clock transition 1 - 2 which is the transition between states of zero total angular momentum. It is forbidden in the absence of hyperfine structure (see, e.g. [16]) or of external field. For that reason the ^{171}Yb isotope which has nuclear spin $I = 1/2$ is usually used for the clock. However, we note that it has recently been shown that a high clock accuracy can also be reached with $I = 0$ (even) isotopes for the $^1\mathrm{S}_0$ - $^3\mathrm{P}_0^\mathrm{o}$ transition [29–31].

In the context of the present study, we do not consider odd isotopes, since in the states 4 and 5 they only possess $J_z \neq 0$ sub-states with very large (electronic) linear Zeeman effect.

Since we need at least four isotopes, there are the following possibilities: (1) Use only M2 clock transitions (transitions 1 - 4 and 1 - 5) in even isotopes. (2) Use magnetic-field induced spectroscopy of the $^1\mathrm{S}_0$ - $^3\mathrm{P}_0$ transition in the four even isotopes with no nuclear spin. Use either of the two M2 transitions as the second clock transition, in the same isotopes.

III. CONCLUSION.

We proposed two new clock states in Yb for use as clock transitions in an optical lattice clock for fundamental research. The transitions are from the ground state to metastable states with easily accessible excitation energies of 19710.388 $\mathrm{cm^{-1}}$ and 23188.518 $\mathrm{cm^{-1}}$ and total angular momentum $J = 2$. Both transitions have all features of optical clock transitions with potential for high accuracy of the frequency measurements. They can also

be used for a search for new physics beyond the Standard Model via studying possible non-linearity of King's plot and testing for a time drift of the ratio of the frequencies. Of course, the transitions could also serve for time keeping. The preparation of the Yb atoms in the optical lattice can be implemented experimentally with the already well-established methods. Their interrogation via M2 excitation would be a novel experimental approach but the appropriate laser could be developed using existing technology. The de-excitation of the atoms from the upper clock state could be done via intermediate excitation to the $4f^{14}6s6d$ states [28]. Thus, it appears that key aspects of the present proposal can be readily characterized on existing clock devices.

When our work was completed a paper by Safronova *et al* [32] on a similar subject appeared in the arXiv. The authors consider another clock transition in Yb, which is the transition between states 2 and 5 in our Table I, and suggest it for searching for time variation of the fine structure constant. There is some overlap between the subjects of the two works and generally reasonably good agreement between overlapping results. E.g., the sensitivity of state 5 to variation of the fine structure constant found in both works is in very good agreement. There are some differences too, in particular in values of the M1 transition amplitudes and the lifetime of the clock state number 5. These differences do not affect the conclusions of both works.

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Appendix A: Calculations of energies, transition amplitudes and polarizabilities.

We perform atomic structure calculations with the CIPT method [12]. It combines configuration interaction (CI) with the perturbation theory (PT) by treating excited configurations perturbatively rather than including them into the CI matrix. This reduces the size of the CI matrix for the many-electron problem by many orders of magnitude, making it possible to deal with systems having a large number of electrons outside closed shells. This is important for the current problem because we are dealing with states of ytterbium which have excitations from the $4f$ subshell. This means that the total number of external electrons is sixteen; e.g., in the excited $4f^{13}5d6s^2$ $(7/2,3/2)_2$ state we have thirteen $4f$ electrons, one $5d$ electron and two $6s$ electrons.

To calculate transition amplitudes we need to include the interaction of the atom with an external electromagnetic field. We consider the interaction in dipole and quadrupole approximation leading to electric and magnetic dipole (E1 and M1) and electric and magnetic quadrupole (E2 and M2) transitions.

We use the random-phase approximation (RPA) for the interaction. The RPA equations for single-electron atomic states have the form

$$(H^{\rm HF}-\epsilon_c)\delta\psi_c=-(\hat{F}+\delta V^F), \tag{A1}$$

where $H^{\rm HF}$ is the Hartree-Fock Hamiltonian, the index c enumerates states in the atomic core, $\delta\psi_c$ is a correction to the core state due to an external field, $\hat{F}$ is the operator of the external field, and δV^F is the correction to the self-consistent Hartree-Fock potential due to the external field. Equations (A1) are solved self-consistently for all states in the core, leading to the effective operator of the external field, $\hat{F}\to\hat{F}+\delta V^F$. Matrix elements between states containing external electrons are calculated by the formula

$$A_{ab}=\langle b||\hat{F}+\delta V^F||a\rangle, \tag{A2}$$

where $|a\rangle$ and $|b\rangle$ are many-electron (sixteen for Yb) wave functions found in the CIPT calculations.

We consider interaction of atomic electrons with external field in dipole and quadrupole approximation leading to electric and magnetic dipole (E1 and M1) and electric and magnetic quadrupole (E2 and M2) transitions.

The rates of spontaneous emission are given in atomic units by

$$R_{E1,M1}=\frac{4}{3}(\alpha\omega)^3\frac{A^2_{E1,M1}}{2J+1}, \tag{A3}$$

for electric dipole (E1) and magnetic dipole (M1) transitions, and by

$$R_{E2,M2}=\frac{1}{15}(\alpha\omega)^5\frac{A^2_{E2,M2}}{2J+1}, \tag{A4}$$

for electric quadrupole (E2) and magnetic quadrupole (M2) transitions. In these formulae α is the fine structure constant, ω is the frequency of the transition in atomic units, A is the amplitude of the transition in atomic units, and J is the total angular momentum of the upper state. The magnetic amplitudes A_{M1} and A_{M2} are proportional to the Bohr magneton $\mu=|e|\hbar/2mc$. Its value in the Gaussian-based atomic units is $\mu=\alpha/2\approx 3.6\times10^{-3}$.

The calculated amplitudes and corresponding transition rates are presented in Table II. Note that the value of the electric dipole transition amplitude between states number 1 (ground state) and state number 10 (which is one of the transitions used for laser cooling of the Yb atom), $\langle 1||E1||10\rangle=4.14$ a.u., is in excellent agreement with the experimental value of 4.148(2) a.u. [13]. This is in sharp contrast to the large disagreement between experiment and the value of 4.825 a.u. obtained in very sophisticated calculations treating the Yb atom as a

two-valence-electron system [15]. The reason for this disagreement is the strong mixing between the $4f^{14}6s6p\ ^1\mathrm{P}^{\mathrm{o}}_1$ and $4f^{13}5d6s^2\ (7/2,5/2)^{\mathrm{o}}_1$ states (states number 10 and 12 in Table I). This mixing cannot be properly taken into account in the two-valence-electrons approximation. See Ref. [15] for a detailed discussion. In current CIPT calculations we explicitly include mixing between three odd configurations, $4f^{14}6s6p$, $4f^{14}5d6p$, and $4f^{13}5d6s^2$, while all other configurations are included perturbatively.

The electric dipole amplitude between two states a and b induced by a magnetic field is

$$A_{\mathrm{B,ab}} = \left(\sum_n \frac{\langle b|M1|n\rangle\langle n|E1|a\rangle}{E_b - E_n} + \sum_n \frac{\langle b|E1|n\rangle\langle n|M1|a\rangle}{E_a - E_n} \right) \times B. \qquad \text{(A5)}$$

Here B is the magnetic field directed along the z axis. The z components of the electric dipole and magnetic dipole matrix elements are used; the summation goes over the complete set of intermediate states. In the SI system, the atomic unit for magnetic field is 1 a.u.$= 2.35\times10^5$ T. The transition rate is given by (A3) while the angular frequency of the Rabi oscillations is $\Omega_R = E_0 A_{\mathrm{B,ab}}$. Here E_0 is the amplitude of the laser electric field. Considering the $^1\mathrm{S}_0$ - $^3\mathrm{P}^{\mathrm{o}}_0$ (1 - 2) transition and using amplitudes from Table II for the three first contributions to (A5) we find that in SI units $\Omega_R/2\pi = (242\ \mathrm{Hz/T}\sqrt{\mathrm{mW/cm^2}})B\sqrt{I}$. Here, I is the intensity of the laser wave. The coupling coefficient is in good agreement with the value $186\ \mathrm{Hz/T}\sqrt{\mathrm{mW/cm^2}}$ from Ref. [18].

The dynamic scalar dipole polarizability of the atom in state $|a\rangle$ when excited by a field of frequency ω_L is given by

$$\alpha_0(\omega_L) = \frac{2}{3(2J_a+1)} \sum_n \frac{E_n - E_a}{(E_n - E_a)^2 - \omega_L^2} \langle a||\hat{D}||n\rangle^2, \qquad \text{(A6)}$$

where the summation goes over the complete set of excited many-electron states, $\hat{D}$ is the operator of the electric dipole interaction in the valence space, $\hat{D} = \sum_v (d_v + \delta V_v)$. Here $d_v = -er_v$, δV_v is the RPA correction to the electric dipole operator acting on electron v (see (A1,A2)), and the summation over v is the summation over the valence electrons.

The total polarizability of a state with angular momentum $J \geq 1$ includes tensor polarizability α_2

$$\alpha(\omega_L) = \alpha_0(\omega_L) + \frac{3J_z^2 - J(J+1)}{J(2J-1)} \alpha_2(\omega_L), \qquad \text{(A7)}$$

where M is projection of J. The expression for $\alpha_2(\omega_L)$ differs from (A6) by the angular coefficient only. The full expression can be found e.g. in Ref. [20]. The method of calculation is described in detail in Ref. [15].

For the effect of the black-body radiation on the clock frequency it is sufficient to consider the scalar polarizabilities at $\omega_L = 0$. On the other hand, to exclude the effect of the laser lattice field on the frequency of the clock transition one needs to find the value of the frequency (magic frequency) at which the polarizabilities of the clock state and of the ground state are the same. For the states 4 and 5 both scalar and tensor polarizability and magic frequencies for the 1 - 4 and 1 - 5 transitions will depend on the projection J_z. We perform such calculations for state 4 while the more complicated case of state 5 is left for future work.

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