^{171}Yb^{+} Single-Ion Optical Frequency Standard at 688 THz

Chr. Tamm, B. Lipphardt, H. Schnatz, R. Wynands, S. Weyers, T. Schneider, and E. Peik

***Abstract*—Two ^{171}Yb^{+} single-ion optical frequency standards operating at 688 THz (436 nm) are compared in order to investigate systematic frequency shifts in the subhertz range. In the absence of externally applied perturbations, a mean relative frequency difference of $3.8 \cdot 10^{-16}$ is observed. Using a femtosecond frequency comb generator based on an Er^{3+}-doped fiber laser, the frequency of the ^{171}Yb^{+} standard is measured with a relative systematic uncertainty of $3.1 \cdot 10^{-15}$ and a statistical uncertainty of $0.6 \cdot 10^{-15}$.**

***Index Terms*—Ion traps, optical atomic clocks, optical frequency measurement, ytterbium-171.**

I. INTRODUCTION

A SINGLE laser-cooled ion in a radio frequency (RF) trap is a nearly ideal reference for an optical frequency standard. For a number of atomic systems, one expects that systematic shifts of the atomic transition frequency can be reduced to the 10^{-18} range (for example, see [1]), which would improve by more than two orders of magnitude on the best available cesium fountain frequency standards. Optical frequency conversion techniques based on femtosecond comb generators permit the realization of practical single-ion frequency standards with output frequencies in the optical and microwave range.

In this paper, we report recent investigations on the 688-THz ^{171}Yb^{+} frequency standard that is based on the $^2S_{1/2}(F = 0) - {}^2D_{3/2}\ (F = 2,\ m_F = 0)$ electric quadrupole transition at 436 nm [2]. This system and single-ion optical frequency standards based on ^{199}Hg^{+} and ^{88}Sr^{+} are presently under review at the International Bureau of Systems and Measures (BIPM), Sèvres, France, as potential secondary representations of the International System of Units (SI) second [3].

In order to overcome the accuracy and stability limitations associated with measurements relative to a microwave frequency reference, we compare two ^{171}Yb^{+} standards directly and observe their frequency difference with and without externally applied perturbations. The tensorial quadratic Stark shift and the quadrupole shift caused by static electric fields are investigated by determining the frequency difference for various orientations of the applied static magnetic field. In the absence of perturbations caused by external static electric fields, we find no evidence of magnetic-field-orientation-dependent shifts larger than the statistical comparison uncertainty of $6 \cdot 10^{-16}$.

These observations enabled absolute measurements of the ^{171}Yb^{+} reference transition frequency with a systematic uncertainty contribution of the ^{171}Yb^{+} standard that is significantly smaller than in previous measurements [4], [5]. In the recent measurements, long continuous averaging intervals of up to 36 h were realized with the use of an Er^{3+}-doped fiber laser comb generator [6], thus significantly reducing the statistical measurement uncertainty associated with the instability of the Cs fountain reference. The results of the new measurements are consistent with our previous results and yield the ^{171}Yb^{+} transition frequency with a statistical uncertainty of $0.6 \cdot 10^{-15}$ and a systematic uncertainty of $3.1 \cdot 10^{-15}$.

II. EXPERIMENTAL SYSTEM

The experiments use two RF Paul traps of identical design with ring electrode diameters of 1.4 mm. The ion is confined by an approximately cylindrically symmetric pseudopotential with an axial depth of 17 eV. In order to compensate any electric stray field at the location of the ion, compensation voltages are applied between the trap endcaps and to two additional electrodes. They are adjusted so that a laser-cooled ion does not change its position by more than 2 μm when the trap potential is lowered to less than 0.25 eV. The remaining stray-field-induced displacement of the ion under normal operating conditions is then calculated to be less than 100 nm.

The ion is laser-cooled to the Lamb–Dicke regime by a frequency-doubled diode laser emitting at 370 nm. Metastable levels that are populated during laser cooling are depleted by diode laser radiation at 935 and 639 nm [7], [8]. The reference transition, which has a natural linewidth of 3.1 Hz, is probed by the frequency-doubled radiation from an 871-nm diode laser locked to a high-finesse cavity. The ^{171}Yb^{+} reference transition can be resolved with a linewidth of 10 Hz [5].

In the frequency comparison experiments, two ^{171}Yb^{+} traps and two independent frequency shift and servo systems are employed to stabilize the probe beam frequencies to the line centers of the reference transitions of the two trapped ions [2]. In order to minimize servo errors due to drift of the probe laser frequency, second-order servo algorithms are used [9]. For averaging times larger than the servo time constants ($\approx$10 s), the optical frequencies probing the two ions can be regarded as independent and determined solely by the respective atomic transition frequencies. The difference Δ of the frequency shifts introduced by the servos is recorded. The ions are interrogated

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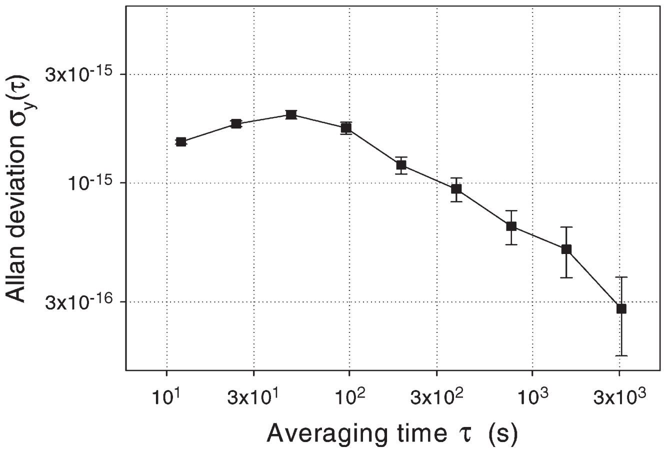

Fig. 1. Allan deviation σ_y of the relative frequency difference Δ/ν between two $^{171}\mathrm{Yb}^+$ single-ion optical frequency standards at $\nu = 688$ THz.

every 90 ms by 30-ms pulses so that the atomic resonance signals have essentially Fourier-limited linewidths of approximately 30 Hz. The relative instability of Δ measured by the Allan standard deviation under these conditions is shown in Fig. 1. The dynamic response of the servo systems leads to a maximum of the Allan deviation at $\tau \approx 50$ s. The observed stability of Δ is independent of the temporal overlap of the probe pulses applied to the two ions, and it is not the result of an exact matching of the time constants of the two servo systems. It is in good agreement with numerical simulations of the servo action, which assume quantum projection noise as the only noise source [9].

III. QUADRUPOLE SHIFT

In most of the presently investigated single-ion optical frequency standards, a significant systematic uncertainty contribution can arise from the interaction of the atomic electric quadrupole moment with the gradient of the electric stray field. In order to cancel the quadrupole shift, one can make use of the fact that the shifts observed for three mutually orthogonal orientations of the magnetic quantization field add up to zero [10], [11]. Alternatively, the quadrupole shift can be canceled by determining the quadrupole shifts of all magnetic sublevels of the reference transition [12].

To investigate the quadrupole shift of the $^{171}\mathrm{Yb}^+$ reference transition, we apply a static electric field gradient A_{dc} in one trap by superimposing a dc voltage on the RF trap drive voltage. The resulting transition frequency shift is measured relative to the other trap operating without dc voltage. Fig. 2 shows the frequency differences observed for various magnetic field orientations in both traps. The data shown are corrected for differences in the quadratic Zeeman shift, which was kept in the range of 0.1–0.5 Hz. The field orientations 1, 2, and 3 are approximately orthogonal to each other with estimated uncertainties of 20° (trap 1) and 10° (trap 2). In order to determine the electric quadrupole moment $\theta(^2\mathrm{D}_{3/2})$ of the upper level of the $^{171}\mathrm{Yb}^+$ reference transition (for the $^2\mathrm{S}_{1/2}$ ground state, $\theta = 0$), the magnetic field orientation was adjusted perpendicular to the trap axis so that the quadrupole shift assumes a local maximum. The corresponding measurement is labeled (1, 4) in Fig. 2. From this, the quadrupole moment is determined as $\theta(^2\mathrm{D}_{3/2}) = 9.32(48) \cdot 10^{-40}\ \mathrm{C \cdot m^2}$, which is in good agreement with the value $9.754 \cdot 10^{-40}\ \mathrm{C \cdot m^2}$ obtained in recent atomic-structure calculations [13].

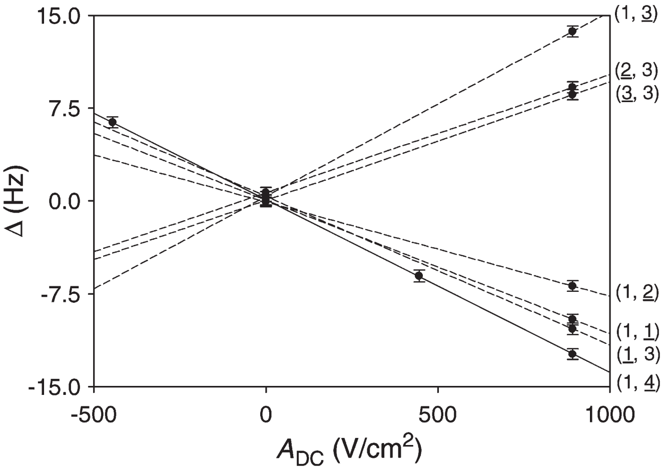

Fig. 2. Frequency difference Δ between the traps as a function of applied electric field gradient A_{dc} for various orientations of the magnetic field in trap 1 and trap 2. The numbers in brackets label the combinations of magnetic field orientations (trap 1, trap 2), and the underlines indicate in which trap the field gradient is applied. Orientations 1, 2, and 3 are approximately orthogonal sets, whereas orientation 4 is perpendicular to the symmetry axis of the trap. The error bars denote the statistical uncertainty of the individual frequency comparisons, and the lines are the results of linear regressions.

IV. QUADRATIC STARK SHIFT

The quadratic Stark shift of the $^{171}\mathrm{Yb}^+$ reference transition has contributions from the scalar polarizability of the ground state, i.e., $\alpha_{\mathrm{S}}(^2\mathrm{S}_{1/2})$, and from the scalar and tensorial polarizabilities of the $^2\mathrm{D}_{3/2}$ state, i.e., $\alpha_{\mathrm{S}}(^2\mathrm{D}_{3/2})$ and $\alpha_{\mathrm{T}}(^2\mathrm{D}_{3/2})$. The dependence of the tensorial Stark shift on the orientation of the magnetic quantization field is analogous to the quadrupole shift. In order to determine $\Delta\alpha_{\mathrm{S}} = \alpha_{\mathrm{S}}(^2\mathrm{S}_{1/2}) - \alpha_{\mathrm{S}}(^2\mathrm{D}_{3/2})$ and $\alpha_{\mathrm{T}}(^2\mathrm{D}_{3/2})$, we determine Δ for the case that in one of the traps, a variable offset is added to the compensation voltage applied between the trap endcap electrodes so that the ion is exposed to the oscillating trap field. The polarizabilities $\Delta\alpha_{\mathrm{S}}$ and $\alpha_{\mathrm{T}}(^2\mathrm{D}_{3/2})$ can then be inferred from measurements with different orientations of the magnetic field.

The results of these measurements are shown in Fig. 3. The data shown are corrected for differences in the quadratic Zeeman shift. The data taken at $\Delta z \neq 0$ are also corrected for the calculated second-order Doppler shift, which amounts to -0.35 Hz at $\Delta z = 1.1\ \mu\mathrm{m}$. At $\beta = 90°$, no significant shift is observed, indicating an accidental cancellation of the scalar and tensorial shift contributions at this angle. From the experimental data, we obtain $\Delta\alpha_{\mathrm{S}} = -6.9(1.4) \cdot 10^{-40}\ \mathrm{J \cdot m^2 \cdot V^{-2}}$ and $\alpha_{\mathrm{T}}(^2\mathrm{D}_{3/2}) = -13.6(2.2) \cdot 10^{-40}\ \mathrm{J \cdot m^2 \cdot V^{-2}}$. These results are close to the polarizabilities $\Delta\alpha_{\mathrm{S}} = -5.20(16) \cdot 10^{-40}\ \mathrm{J \cdot m^2 \cdot V^{-2}}$ and $\alpha_{\mathrm{T}}(^2\mathrm{D}_{3/2}) = -12.13(13) \cdot 10^{-40}\ \mathrm{J \cdot m^2 \cdot V^{-2}}$, which were inferred from computed oscillator strengths and experimental lifetime data [14].

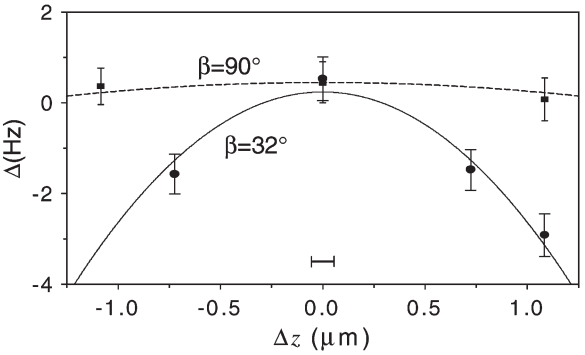

Fig. 3. Frequency difference Δ between the traps as a function of the displacement Δz of the ion in trap 2 from the saddle point of the RF trap potential. β denotes the angle between trap axis and magnetic field, as inferred from the quadrupole shift measurements shown in Fig. 2. The lines are least square fits of parabolas centered at $\Delta z = 0$. The horizontal bar in the lower part of the figure denotes the uncertainty range of the position $\Delta z = 0$, which remains after the compensation of the electric stray field.

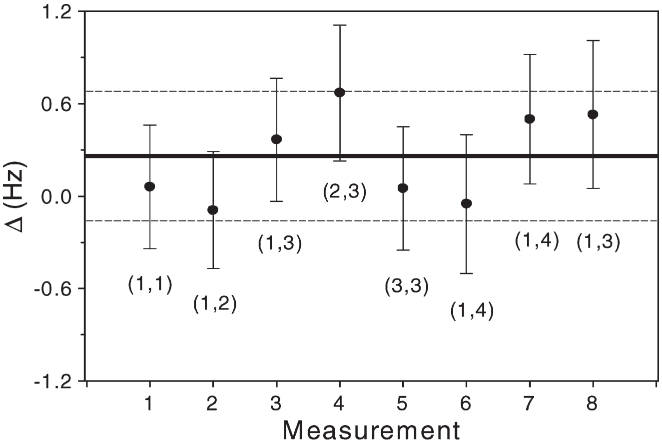

Fig. 4. Frequency difference in the absence of external perturbations, showing the data points of Fig. 2 at $A_{\mathrm{dc}} = 0$ (measurements 1–6) with two more data points added. The data were taken within 2 days and are displayed in a temporal order. The solid line is the weighted average of the data, and the dashed lines mark the average statistical uncertainty of the data points.

V. AGREEMENT BETWEEN TRAPS

Fig. 4 shows measurements of the frequency difference Δ for $A_{\mathrm{dc}} = 0$ and $\Delta z = 0$ in both traps. The weighted mean difference of all eight measurements is $\langle\Delta\rangle = 0.26$ Hz, and the average statistical uncertainty is 0.42 Hz. The contribution of the quadratic Zeeman shift to the systematic uncertainty of Δ is smaller than 0.05 Hz. Using a stray-field compensation procedure as previously described, the uncertainty contribution from quadratic Stark and second-order Doppler shift is below 0.02 Hz [15]. The blackbody ac Stark shift expected from the measured static polarizability $\Delta\alpha_{\mathrm{S}}$ is $-0.37(5)$ Hz at 300 K. Additional ac Stark shifts due to ambient heat sources and laser stray light are estimated to be smaller than 0.3 Hz. The uncertainty contribution resulting from servo errors is smaller than 0.1 Hz [9].

A χ^2 test indicates that within the statistical uncertainty of the data shown in Fig. 4, there is no evidence of frequency shifts that depend on the orientation of the magnetic quantization field [15]. This permits the conclusion that stray-field-induced quadrupole shifts were smaller than 0.5 Hz under the conditions of the measurement. For an uncertainty estimate on the observed mean frequency difference $\langle\Delta\rangle = 0.26$ Hz, it would appear justified to regard the scatter of the data as random. Nevertheless, as it is difficult to determine the contribution of residual systematic shifts to the scatter of the data points, we estimate the uncertainty of $\langle\Delta\rangle$ as the average statistical uncertainty of the data points.

TABLE I

SUMMARY OF RECENT RESULTS OF ABSOLUTE FREQUENCY MEASUREMENTS OF THE ^{171}Yb^{+} STANDARD. THE TRANSITION FREQUENCIES ν_i ARE CORRECTED FOR THE QUADRATIC ZEEMAN SHIFT PRESENT DURING THE MEASUREMENTS. BLACKBODY SHIFT CORRECTIONS (SEE SECTION V) ARE NOT APPLIED. THE 1σ STATISTICAL UNCERTAINTIES OF THE MEASUREMENTS ARE DENOTED BY $u_{\mathrm{A}i}$. THE 1σ SYSTEMATIC UNCERTAINTY CONTRIBUTIONS OF THE ^{171}Yb^{+} STANDARD AND OF THE CESIUM FOUNTAIN REFERENCE ARE DENOTED BY u_{B} (Yb^{+}) AND u_{B} (Cs), RESPECTIVELY. ALL UNCERTAINTY DATA ARE SCALED TO THE FREQUENCY OF THE ^{171}Yb^{+} STANDARD (688 THz)

ν_i = 688 358 979 309 000 + x_i Hz; i: number of measurement

i	Starting Date	x_i (Hz)	$u_{\mathrm{A}i}$ (Hz)	u_{B}(Cs) (Hz)	u_{B}(Yb^{+}) (Hz)
1	5.7.2005	307.84	3.43	1.82	1.05
2	6.7.2005	307.51	0.46	1.82	1.05
3	9.8.2005	307.49	1.01	1.82	1.05
4	10.8.2005	307.07	0.64	1.82	1.05
5	22.6.2006	307.70	0.44	1.82	1.05

Weighted mean including earlier results (Ref. 5):

$\nu[^{171}\mathrm{Yb}^{+}, {}^{2}S_{1/2}(F=0) - {}^{2}D_{3/2}(F=2)]$ = 688 358 979 309 307.6(2.2) Hz

VI. ABSOLUTE FREQUENCY MEASUREMENT

For the absolute frequency measurements, the second harmonic of the probe laser frequency is stabilized to the reference transition of a trapped ^{171}Yb^{+} ion. A part of the 871-nm probe laser output is passed through an 8-m fiber link to produce a beat signal with the frequency-doubled output of an Er^{3+}-doped fiber frequency comb generator [6]. The comb generator is referenced to the primary cesium fountain frequency standard CSF1 of Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany.

The trap employed for the frequency measurements was operated without externally applied perturbations and with a constant orientation of the magnetic quantization field. The measurements were performed at an ambient temperature of 296 K. A comparison between the two traps was carried out immediately before one absolute frequency measurement interval and yielded results consistent with those shown in Fig. 4.

Five absolute frequency measurements with continuous averaging times of up to 36 h were conducted between July 2005 and June 2006. The results are listed in Table I. The obtained statistical measurement uncertainties are dominated by the white frequency noise of the Cs fountain reference. The systematic uncertainty contribution of the Cs reference takes into account that a new uncertainty evaluation of CSF1 was incomplete at the time of the measurements. The systematic uncertainty of the $^{171}\mathrm{Yb}^+$ standard is dominated by the contribution from the stray-field-induced quadrupole shift. In this paper, an uncertainty of 1 Hz is assumed, which is approximately a factor of two larger than the statistical uncertainty of the frequency comparison measurements shown in Fig. 4.

The frequency measurements described in this paper are in excellent agreement with our earlier results [4], [5]. The individual results contribute to the mean frequency ν noted in Table I with weights proportional to $(\mathrm{u}_{\mathrm{Ai}}^2 + \mathrm{u}_{\mathrm{B}}^2(\mathrm{Cs}) + \mathrm{u}_{\mathrm{B}}^2(\mathrm{Yb}^+))^{-1}$. The total 1σ uncertainty of ν is calculated as $\mathrm{u} = (\mathrm{u}_{\mathrm{A}}^2 + \mathrm{u}_{\mathrm{B}}^2(\mathrm{Cs}) + \mathrm{u}_{\mathrm{B}}^2(\mathrm{Yb}^+))^{1/2}$ with $\mathrm{u}_{\mathrm{A}} = (\Sigma_{\mathrm{i}}(\mathrm{u}_{\mathrm{Ai}})^{-2})^{-1/2}$, which yields $\mathrm{u} = 2.2$ Hz. The corresponding relative statistical and systematic uncertainties are $\mathrm{u}_{\mathrm{A}}\ \nu^{-1} = 0.6 \cdot 10^{-15}$ and $(\mathrm{u}_{\mathrm{B}}^2(\mathrm{Cs}) + \mathrm{u}_{\mathrm{B}}^2(\mathrm{Yb}^+))^{1/2}\ \nu^{-1} = 3.1 \cdot 10^{-15}$, respectively.

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