Evaluation of blackbody radiation shift with temperature-associated fractional uncertainty at $10^{-18}$ level for $^{40}\text{Ca}^+$ ion optical clock

Ping Zhang$^{1,2,3,4}$, Jian Cao$^{1,2,5}$, Hua-lin Shu$^{1,2}$, Jin-bo Yuan$^{1,2,3}$, Jun-juan Shang$^{1,2,3}$, Kai-feng Cui$^{1,2,3}$, Si-jia Chao$^{1,2,3}$, Shao-mao Wang$^{1,2,3}$, Dao-xin Liu$^{1,2,3}$ and Xue-ren Huang$^{1,2,5}$

$^1$ State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, People’s Republic of China
$^2$ Key Laboratory of Atom Frequency Standards, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, People’s Republic of China
$^3$ University of Chinese Academy of Sciences, Beijing 100049, People’s Republic of China
$^4$ School of Physics and Electrical Engineering, Taizhou University, Taizhou 318000, People’s Republic of China

E-mail: caojian@wipm.ac.cn and hxueren@wipm.ac.cn

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Abstract
In this paper, the blackbody radiation (BBR) temperature rise experienced by a $^{40}\text{Ca}^+$ ion confined in a miniature Paul trap and its uncertainty have been evaluated via finite-element method (FEM) modelling. The FEM model was validated through comparisons with thermal camera measurements at several points on a dummy trap. Before the validation, the thermal camera was calibrated by using a PT1000 resistance thermometer. The input modelling parameters were analyzed carefully, and their contributions to the uncertainty of the trap environment temperature were evaluated using the validated FEM model. The result shows that the temperature rise experienced by the $^{40}\text{Ca}^+$ ion is 1.72 K with an uncertainty of 0.46 K. It results in a contribution of 2.2 mHz to the systematic uncertainty of a $^{40}\text{Ca}^+$ ion optical clock, corresponding to a fractional uncertainty $5.4 \times 10^{-18}$. This is much smaller than the uncertainty caused by the BBR shift coefficient, which is evaluated to be 4.8 mHz and at the $10^{-17}$ level in fractional frequency units.

Keywords: blackbody radiation shift, temperature rise evaluation, $^{40}\text{Ca}^+$ ion optical clock, systematic uncertainty

(Some figures may appear in colour only in the online journal)

1. Introduction

Optical clocks, based both on single trapped ions [1–4] and neutral atoms [5–8], have demonstrated great improvements in recent years. Some of them have been confirmed to be more accurate than the Cs microwave frequency standards which are currently realized as the SI second [3–6]. However, there are a number of systematic shifts that still need to be overcome and one of them is blackbody radiation (BBR) shift, which has been identified as one of the largest contributions to the systematic uncertainty for many optical clocks. In particular, in single ion optical clocks which trap the ion using a radio frequency (RF) field, heating is unavoidable due to RF absorption in the insulators and joule
heating in the conductors. Thus, it is more difficult to evaluate temperature precisely for ion optical clocks compared with those using neutral atoms confined in optical lattices.

Optical clocks based on the $^{40}$Ca$^+$ ion have been well developed in the past decades due their advantages of having a relatively simple scheme and low cost [2, 9, 10]. However, unlike the one based on $^{27}$Al$^+$ ion which is insensitive to BBR [1], $^{40}$Ca$^+$ ion optical clocks possess a large BBR shift which contributes a lot to the clock systematic uncertainty [2]. It has been identified that the uncertainty of BBR shift is basically dependent on the uncertainty of the BBR shift coefficient and the uncertainty of temperature measurement on the trap environment [11]. For a $^{40}$Ca$^+$ ion optical clock based on $4s_{1/2}$-$3D_{3/2}$ transition, the first part is the uncertainty of the differential scalar polarizability of $4s_{1/2}$ and $3D_{3/2}$ states, which results in a contribution of fractional frequency uncertainty at the $10^{-17}$ level according to the theoretical calculations described in [11]. The latter is strongly limited by the accuracy of experimental measurements of the trap environment temperature and also has a contribution at the $10^{-17}$ level in fractional frequency units when measured using temperature sensors [1, 12] or thermal imaging devices [2, 4]. Recently, trap temperature has been evaluated more precisely via a method based on finite-element method (FEM) modelling [13, 14]. The results indicate that the temperature-associated fractional uncertainty of BBR shift has the potential to reach the $10^{-18}$ level and will no longer be one of the largest contributors to the systematic uncertainty for most ion optical clocks.

Here, we evaluate the BBR temperature rise seen by a $^{40}$Ca$^+$ ion in a miniature Paul trap via FEM modelling. For validating the FEM model, a dummy trap was established and the model validated by comparing the modeling results with the temperature of the dummy trap in a vacuum chamber measured by using a thermal camera. To obtain the actual temperature, the thermal camera was calibrated by PT1000 in advance. The uncertainty of input modelling parameters and their contributions to the uncertainty of the BBR temperature rise were evaluated in detail subsequently. The evaluation result indicates that the temperature rise seen by the $^{40}$Ca$^+$ ion is 1.72 K with an uncertainty of 0.46 K. It causes a contribution of 2.2 mHz to the systematic uncertainty and $5.4 \times 10^{-18}$ in fractional frequency units. Compared to the one caused by the BBR shift coefficient at the $10^{-17}$ level, this uncertainty is much smaller and no longer one of the main contributions to the total BBR shift uncertainty of the $^{40}$Ca$^+$ ion optical clock.

2. Trap description and BBR FEM modelling

The miniature Paul trap has been used in $^{40}$Ca$^+$ ion optical clock studies at the Wuhan Institute of Physics and Mathematics in China (WIPM) for many years [2, 15, 16]. The improved structure of the miniature Paul trap employed in our system is shown in figure 1. This trap contains one ring electrode, two endcap electrodes and two compensation electrodes. These electrodes are all made from molybdenum.

![Figure 1. Structure of miniature Paul trap. This kind of trap contains one ring electrode, two endcap electrodes and two compensation electrodes which are connected to titanium wires on a titanium support disc through spot welding.](image)

The radius of the ring electrode wire is 0.25 mm, and that of the endcap electrode wires as well as the potential electrode wires is 0.5 mm. The ratio of these two radii was optimized to be 0.5 mm in our previous work [15]. All of these electrodes are connected to titanium wires on a titanium support disc. To obtain good electronic and thermal connections, they are fixed together through spot welding. Then, titanium support discs are mounted to a vacuum feedthrough. Both electronic and thermal connections between their electrodes are also achieved through spot welding. The ceramics used in the support disc and the vacuum feedthrough to insulate the electrodes from them are both alumina.

An FEM model using the COMSOL Multiphysics software package was developed to evaluate the temperature rise of the trap system and the radiation temperature rise seen by the $^{40}$Ca$^+$ ion. In the model, the electromagnetic waves (frequency domain) found under the radio frequency (RF) branch are employed to study the electric field and the heat transfer in solid found under the heat transfer branch is used to study the thermal distribution. RF absorption in insulators and joule heating in conductors are regarded as the two main sources of heat generation, and radiation and conduction in solids are the two primary sources of heat removal. A small blackbody sphere with unity emissivity and a thermal conductivity of 1000 W m$^{-1}$ K$^{-1}$ was located at the center of the ring electrode to evaluate the radiation temperature rise there. The diameter of the sphere is 10 μm, and the temperature fluctuation on it could be neglected due to its high thermal conductivity. In modelling, a 24.5 MHz RF was added between the ring electrode and the endcap electrodes according to the one used to trap the $^{40}$Ca$^+$ ion in our optical clock system. The zero-to-peak RF amplitudes are 520 V and 700 V for validating the model and evaluating the temperature rise, respectively. In the trap system, besides molybdenum, titanium, and alumina mentioned above, titanium and fused silica were also used at the vacuum chamber and windows. The main properties of the materials used in FEM modelling are listed in table 1.
Table 1. The main properties of materials used in FEM modelling.

| Material       | Electrical conductivity$^a$ (MS m$^{-1}$) | Thermal conductivity (W m$^{-1}$ K$^{-1}$) | Emissivity | Relative permittivity$^a$ | Dielectric loss tangent$^a$ |
|----------------|------------------------------------------|------------------------------------------|------------|--------------------------|---------------------------|
| Molybdenum     | 17.6                                     | 139                                      | 0.162      | —                        | —                         |
| Titanium       | 1.82                                     | 21                                       | 0.166      | —                        | —                         |
| Aluminum       | 36.0                                     | 150                                      | 0.25       | —                        | —                         |
| Alumina        | —                                        | 35.4                                     | 0.9        | 9.5                      | 2.0E-4                    |
| Fused silica   | —                                        | 1.35                                     | 0.8        | 3.82                     | 1.5E-5                    |

$^a$ Electrical conductivity of ceramics, relative permittivity and dielectric loss tangent of metals have not been considered in the modelling and assigned by the default value of the finite-element analysis software.

The properties list in this table are mainly referred to in [13] and others which are not listed here are given by the finite-element analysis software by default.

3. Results and discussion

3.1. Validation of the FEM model

The FEM model was validated by comparing it with the measurements of trap temperature at several points on a dummy trap. Experimentally, it is very difficult to measure the trap temperature accurately by using thermal temperature sensors due to the influence of RF. Thus, a thermal camera (Fluke Ti400) ranging from 7.5 um to 14 um, instead of thermal temperature sensors, was employed to gauge the trap temperature in the vacuum chamber through a CaF window. The lower emissivity of molybdenum, as well as the lower transmissivity of the CaF window in the far-infrared range, causes the measurement using thermal camera to deviate from the actual temperature. Moreover, a parameter of low emissivity can make the uncertainty of the measurements larger when using a thermal camera. To avoid such problems, a calibration of the thermal camera measurements was carried out through comparisons with the temperature measured by a calibrated PT1000 resistance thermometer. For getting the actual temperature, a PT1000 resistance thermometer was glued on the molybdenum plate using a silicon heat sink compound. Then the plate together with the thermometer was put into a vacuum chamber to gauge temperature more precisely. For obtaining more data, the plate was heated up by a film heater stuck on the back side at different DC currents. After thermal balance under a fixed heating current, the steady-state temperature of molybdenum was measured by the PT1000 resistance thermometer and the thermal camera simultaneously. The relationship of these two measurements under different steady-state temperatures is exhibited in figure 2. As shown in the figure, the dots are the measured results and the line is obtained by polynomial fitting.

Figure 3 presents the thermal pictures of the miniature Paul trap (a) without an applied RF and (b) with an applied RF. The zero-to-peak amplitude of RF applied on the dummy trap is 520 V determined by a calculation described below. Obviously, the trap temperature in figure 3(b) is higher than the one in figure 3(a). This means the trap structure has been heated up after adding RF between the electrode and the endcap electrodes. The surface of the spot welding region is brighter than the other area. This may be caused by the differences of reflectivity and emissivity between the spot welding material and molybdenum. By using the software included with the thermal camera, the temperatures of the ring and endcap electrodes were determined to be 296.9 K and 296.8 K, respectively. According to the fit line in figure 2, the actual temperature of these two electrodes was estimated to be 300.0 K and 299.6 K. Then, the FEM model was validated by adjusting the structure of the insulator and its thermal conductivity until the modelling results coincided with the measured temperatures.

3.2. Uncertainty estimation of modelling parameters

For evaluation of the temperature rise seen by the ion via FEM modelling, uncertainty mainly arises due to input modelling parameters such as RF amplitude, dielectric loss tangent of ceramic, thermal conductivity of ceramic, emissivity of trap electrodes and inhomogeneous vacuum chamber temperature [13]. According to the structure of the miniature Paul trap and the chosen materials, the main input parameters have been analyzed and estimated conservatively in the following. The value of these parameters and their uncertainty are listed in table 2.

The RF zero-to-peak amplitude of the trap system was measured to be 600 V by using an oscilloscope. This value deviates from the actual voltage amplitude used to trap the $^{40}$Ca$^+$ ion due to the self-capacity of the high-voltage probe in.
respectively, at a different load capacitance. When trapping a

where $\varepsilon = \varepsilon' + j\varepsilon''$, $\varepsilon''$ is the dielectric loss tangent of alumina.

The value of main input parameters and their uncertainty

tabelle used in evaluating the radiation temperature rise seen by the single

Table 2. The value of main input parameters and their uncertainty

| Main parameter               | Value | Uncertainty |
|------------------------------|-------|-------------|
| RF amplitude (V)             | 700   | 50          |
| Emissivity of Mo             | 0.16  | 0.09        |
| Thermal conductivity of alumina (W m$^{-1}$ K$^{-1}$) | 27.5  | 7.5         |
| Dielectric loss tangent of alumina (10$^{-4}$) | 1.5   | 0.5         |
| Initial temperature of electrodes (K) | 292.2 | 1.0         |
| Vacuum chamber temperature (K) | 292.2 | 0.1         |

parallel. To determine the amplitude more precisely, the following calculation was carried out. According to [17], the resonant frequency $f$ of a helical resonator can be calculated from the following equation:

$$ f = \frac{1}{2\pi \sqrt{LC}}, $$  \hfill (1)

where $L$ is the inductance and $C$ is the capacitance of the trapping system. The output voltage $V$ of the helical resonator is

$$ V = \left(\frac{L}{C}\right)^{1/4} \sqrt{PQ}, $$  \hfill (2)

where $P$ is input power and $Q$ is the quality factor. When connecting a different load capacitance, we can get the following relation:

$$ \frac{V}{V'} = \left(\frac{C'}{C}\right)^{1/4} \frac{\sqrt{Q}}{\sqrt{Q'}} \frac{\sqrt{P}}{\sqrt{P'}} = \left(\frac{f'}{f}\right)^{1/2} \left(\frac{Q}{Q'}\right)^{1/2} \left(\frac{P}{P'}\right)^{1/2}, $$  \hfill (3)

where $V'$, $C'$, $Q'$, $P'$, $f'$ are the output voltage, total capacitance, quality factor, input power and resonant frequency, respectively, at a different load capacitance. When trapping a $^{40}\text{Ca}^+$ ion, a tunable capacitance is used to obtain a resonant frequency of about 24.5 MHz. In this case, we assume the output voltage, resonant frequency, quality factor and input power are $V_1, f_1, Q_1, P_1$, respectively. Then, connecting the high-voltage probe, these values are assumed to be $V_2, f_2, Q_2, P_2$, respectively. For the case of using the high-voltage probe and without the tunable capacitance, these values are supposed to be $V_3, f_3, Q_3, P_3$, respectively. Where the output voltage $V_2, V_3$ can be measured by an oscilloscope and the resonant frequency $f_1, f_2, f_3$ can be read out from a function generator. In all cases, the input powers $P_1, P_2, P_3$ are 5 W, respectively. Then from equation (3), we can obtain the value of $(Q_2/Q_3)^{1/2}$. According to [18], it can be considered that the quality factor $Q$ has a linear relationship with the resonant frequency $f$ approximately in a small range. Thus, $(Q_2/Q_3)^{1/2}$ can be determined from the value of $(Q_2/Q_3)^{1/2}$. Subsequently, the value of $V_1$ can be obtained according to equation (3). Finally, based on the calculation described above, the output voltage of the trapping system and the dummy trap are determined to be 700 V and 520 V, respectively. The uncertainties of these two output voltages are evaluated to be 44 V and 48 V, respectively. In modelling, the output voltage uncertainty is considered to be 50 V conservatively.

It can be clearly seen from the modelling results as well as the thermal picture that the temperature of the ring and endcap electrodes made from molybdenum is higher than the other trap structure. Moreover, the surfaces of these electrodes are visible to the $^{40}\text{Ca}^+$ ion. Consequently, the uncertainty of molybdenum emissivity makes a large contribution to the uncertainty of the radiation temperature seen by the ion. According to [13], molybdenum emissivity has been identified to be 0.16. In our work, the emissivity was also estimated to be 0.16 by adjusting the thermal camera measurement of molybdenum according to the temperature of black tape on it. Actually, it is very difficult to evaluate molybdenum emissivity accurately. As the emissivity of most material is determined by surface quality, temperature and wavelength of measurement. According to the technical literature and the user manuals for many thermal imaging systems, for polished, unoxidized or slightly oxidized molybdenum, the emissivity ranges from 0.05–0.24 [19], 0.08–0.26 [20], and 0.06–0.18

\[\text{Figure 3. Thermal images of the miniature Paul trap (a) without an applied RF and (b) with a 520 V RF at about 24.5 MHz.}\]
RF absorption in ceramics has been confirmed to be one of the major heating sources in the trap. The power of heating due to RF absorption has a relation with relative permittivity and the dielectric loss tangent according to the following equation [13]:

\[ p = 2\pi f_0\varepsilon_0\tan(\delta)|E|^2, \]

where \( f \) is the frequency of the electric field, \( \varepsilon_0 \) is the permittivity of free space, \( \varepsilon_r \) is the real relative permittivity and \( \tan(\delta) \) is the dielectric loss tangent. The dielectric loss tangent of alumina is strongly dependent on its composition, processing and purity ranges from \( 1.0 \times 10^{-4} \) to \( 2 \times 10^{-4} \). Thus, \( 1.5 \times 10^{-4} \) and \( 0.5 \times 10^{-4} \) is adopted as the dielectric loss tangent of alumina and its evaluation uncertainty. Moreover, the lower thermal conductivity of ceramics can influence the heat dissipation of the ring electrode and makes a large contribution to the thermal distribution of the trap structure. For commercial alumina ceramics, thermal conductivity ranges from 20 to 35 W m\(^{-1}\) K\(^{-1}\). So, the thermal conductivity and its uncertainty are estimated to be 27.5 W m\(^{-1}\) K\(^{-1}\) and 7.5 W m\(^{-1}\) K\(^{-1}\), respectively.

The temperature of the room and the interior space of the vacuum chamber were monitored for more than 48 h. The room temperature fluctuates by less than 2 K around 292.20 K, while the one in the vacuum chamber fluctuates less than 0.20 K. As the electrodes are separated from the feedthrough by ceramics, their temperatures can be considered to have the same homogeneity as the room temperature. So the minimum and maximum initial temperature of the electrodes can be estimated to be 291.20 K and 293.20 K conservatively. For the ion confined in the vacuum chamber, it can be considered to possess a fluctuant temperature coinciding with the one in the interior space of the vacuum chamber. Namely, it contributes 0.10 K to the uncertainty of the radiation temperature seen by ion.

3.3. Evaluation of temperature rise experienced by the \(^{40}\text{Ca}^+\) ion

Figure 4 shows the modelled temperature distribution of the miniature Paul trap with a 700 V RF at 24.5 MHz. It can be seen that the temperature of the ring electrode together with the middlemost titanium wire is highest, at approximately 306 K. The temperature of the ring and endcap electrodes is determined to be 305.39 K and 304.39 K respectively. From the simulation process, it can be clearly seen that the alumina insulator connected to the ring electrode heats up first. That may mainly be attributed to RF absorption in the insulators, as well as joule heating in the conductors, which have been identified as the two main sources of heat generation in ion traps [13]. Therefore, it is possible to reduce the temperature rise of the ring electrode as well as other electrodes by adopting insulators with a lower dielectric loss tangent and metal electrodes with higher electrical conductivity.

A small ball with blackbody properties was placed at the ion position to evaluate the radiation temperature and its uncertainty seen by the \(^{40}\text{Ca}^+\) ion. The feasibility of this was discussed in [13]. According to whether or not it relates to RF heating, RF heating and fluctuation of room temperature have been taken into account to evaluate the uncertainty of temperature rise, respectively, and the evaluation results are listed in table 3. It can be seen that the temperature rise experienced by the ion caused by RF heating is about 1.72 K and the two largest contributors to the uncertainty come from the emissivity of molybdenum and RF amplitude, which are 0.42 K and 0.13 K respectively. Meanwhile, the contribution of room temperature fluctuation cannot be neglected. Due to fluctuations with room temperature, the initial temperature of the electrodes were regarded to be 291.20 K and 293.20 K, respectively, and contributed 0.06 K to the uncertainty of radiation temperature. Moreover, the temperature fluctuation in the interior space of the vacuum chamber was identified to contribute 0.10 K to the uncertainty of the radiation temperature experienced by the ion. All in all, the radiation temperature rise seen by \(^{40}\text{Ca}^+\) ion in the miniature Paul trap is evaluated to be 1.72 K with an uncertainty of 0.46 K. The achieved temperature accuracy can be mainly attributed to less insulator use, invisibility of the insulator to the ion, the calibration of thermal camera measurements using the PT1000 thermometer and the precise determination of RF voltage amplitude. Furthermore, the structure of the support disc used as a heat sink is also helpful to reduce the temperature rise of the trap and make the evaluation more accurate. According to [11], the temperature-associated contribution to uncertainty of BBR shift is 2.2 mHz, corresponding to a fractional uncertainty 5.4 \( \times \) \( 10^{-18} \). While, the total uncertainty of BBR shift is 5.3 mHz and the uncertainty of the BBR shift coefficient provides a major contribution of 4.8 mHz.
which is at $10^{-17}$ level in fractional units. Obviously, the temperature-associated uncertainty of BBR shift is much smaller than the one caused by the BBR shift coefficient.

### 4. Conclusion

BBR shift has been found to be one of the largest contributors to the systematic uncertainty of $^{40}$Ca$^+$ optical clocks. The BBR temperature rise experienced by the $^{40}$Ca$^+$ ion and its uncertainty were evaluated via FEM modelling. The FEM model was validated by comparing it with the trap temperature at several points on the dummy trap measured by using a thermal camera. The thermal camera measurements were calibrated by using a PT1000 resistance thermometer for obtaining the actual temperature of molybdenum in the vacuum chamber. The uncertainty of input modelling parameters and their contributions to the uncertainty of the radiation temperature rise were evaluated in detail. The evaluation result shows that the radiation temperature rise experienced by the $^{40}$Ca$^+$ ion in the miniature Paul trap is 1.72 K with an uncertainty of 0.46 K. That means it contributes 2.2 mHz and $5.4 \times 10^{-18}$ in fractional units to the BBR shift uncertainty of the $^{40}$Ca$^+$ optical clock. The total uncertainty of BBR shift is 5.3 mHz, which is mainly contributed by the BBR shift coefficient with 4.8 mHz and at $10^{-17}$ level in fractional units.

However, the evaluation has reduced BBR shift uncertainty due to temperature to 2.2 mHz. It could be further improved via optimizing the trap structure. According to the model, the heating originates mainly from RF absorption in insulators and joule heating in conductors. Thus, it is essential to adopt insulators with a lower dielectric loss tangent and metal electrodes with higher electrical conductivity to reduce the temperature rise of electrodes. Moreover, the radiation temperature rise experienced by the ion can be reduced using electrodes with lower emissivity and higher thermal conductivity. Simultaneously, more precise measurements and estimations on the modelling parameters are essential for reducing their contributions to the systematic uncertainty.

Besides the trap environment temperature, the uncertainty of BBR shift is also related to the BBR shift coefficient. Currently, the uncertainty of the BBR shift coefficient is limited by theoretical calculations for the $^{40}$Ca$^+$ ion optical clock based on $4s_{1/2}$-$3D_{5/2}$ transition. This coefficient of $^{88}$Sr$^+$ has reached the level of $10^{-19}$ by a method based on high-accuracy experimental measurements of the differential static scalar polarizability [22]. If a similar approach is used for $^{40}$Ca$^+$, there is a good potential to determine the BBR shift coefficient more accurately. Consequently, the total uncertainty of BBR shift could reach the level of $10^{-18}$ for the $^{40}$Ca$^+$ optical clock in the near future.

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