

# Operational compensation for higher order uncertainties in frequency standards of magnesium and calcium atoms in optical lattices

V.D. Ovsianikov, S.I. Marmo, S.N. Mokhnenko, V.G. Pal'chikov

**Abstract.** The possibilities and ways for operational tuning of optical lattice parameters, which make it possible to minimise the frequency-standard uncertainties caused by nonlinear, nondipole, and anharmonic effects of interaction of magnesium and calcium atoms with the optical lattice field of a magic wavelength, have been investigated.

**Keywords:** atom, electromagnetic radiation, standing wave, magnetic field, polarisability, hyperpolarisability, multipole interaction.

## 1. Introduction

Currently, the atoms belonging to the IIA (Mg, Ca, Sr) and IIB (Zn, Cd, Hg) groups of the Periodic system of elements, as well as rare-earth Yb atoms, are considered to be the most promising objects for designing ultrahigh-precision frequency and time standards of new generation. An attractive feature of these atoms is that they possess a metastable state  $nsnp(^3P_0)$ , whose radiative decay to the ground state  $ns^2(^1S_0)$  corresponds to oscillations of an oscillator with an extremely high  $Q$  factor. The record stability and accuracy of reproducing periods of these oscillations (at a level of a few parts in  $10^{18}$ ) [1–6] stimulate stable interest in the potential of the aforementioned atoms as a base of frequency and time standards. The application of optical lattices with magic wavelengths  $\lambda_{\text{mag}}$ , which have been experimentally measured to date with a high accuracy [7, 8], makes it possible to advance significantly in solving this problem. To this end, consideration of the nonlinear, nondipole, and anharmonic effects of interaction of atoms with the optical-lattice field calls for precise lattice frequency control with introduction of the concept of ‘operational magic frequency’ [9–11].

Since magnesium and calcium atoms are the lightest among the aforementioned atoms, it is more difficult to cool, trap, and confine them in the optical-lattice field as compared with the others. In addition, the low natural content of odd (fermionic) isotopes of these elements (less than 10% for magnesium and less than 0.15% for calcium) with a nonzero magnetic moment of atomic nucleus, which provides magnetically

induced admixture of the  $^3P_1$  state to the metastable state  $^3P_0$ , is a significant hindrance for observing the strongly forbidden line of radiative decay of the metastable state of the isotope. However, this transition can be observed in atoms of bosonic isotopes by applying an external magnetic field, which mixes the  $^3P_0$  and  $^3P_1$  states [12]. In particular, a magnetic field  $B = 100$  G induces a decay of the metastable  $^3P_0$  state in magnesium and calcium atoms at the rate of  $\sim 0.01$  s $^{-1}$ . Thus, a magnetic field may cause a radiative transition (accessible for observation) of an atom from the metastable level to the ground state [13, 14]. The frequency shift (quadratic in  $B$ ) of the clock transition,  $\Delta\nu_{\text{cl}}(B) = -\nu_B B^2$  ( $\nu_B = 2.173$  Hz G $^{-2}$ ), is 21.7 kHz at  $B = 100$  G for Mg atoms. This frequency shift of the standard can be taken into account in measurements with an uncertainty of  $\sim 4$  mHz at  $\Delta B/B \approx 10^{-7}$ ; i.e., with an uncertainty of the magnetic field amplitude  $|\Delta B|$  at a level of 0.01 mG. These estimates show that the necessity of using a magnetic field hinders significantly the development of frequency standards based on bosonic isotopes with record accuracies.

The  $nsnp(^3P_0) \rightarrow ns^2(^3S_0)$  transition is a unique natural oscillator with a maximum attainable  $Q$  factor of oscillation frequency, which is determined by the strength of external magnetic field and the spin–orbit splitting energy in magnesium and calcium atoms. However, the advantage of light atoms, which is provided by the smaller splitting of the triplet states  $^3P_{J=0,1,2}$  into fine-structure sublevels and facilitates their mixing by the magnetic field, is lost to a great extent due to the lower (as compared with heavy atoms) probability of the intercombination transition  $^3P_1 - ^1S_0$ . In addition, the high radiative recoil energies significantly impede the secondary cooling of light atoms and achievement of operating temperatures at a level of few microkelvins, which are necessary for efficient trapping and confining of atoms by optical lattice.

Until now, the aforementioned specific features of magnesium and calcium atoms hindered detailed study of the possibility of their application for designing frequency standards. Nevertheless, theoretical calculations of the magic wavelength for calcium atoms [15] and its approximate estimation based on the single-electron model potential [16] for magnesium atoms and even lighter divalent helium and beryllium atoms were performed more than ten years ago [17–19].

However, the model potential approach, which yields satisfactory results for monovalent alkali metal atoms, turned out to be fairly rough for estimating the susceptibilities of divalent atoms and called for additional modifications. These modifications provide more correct results, which are in satisfactory agreement with the quantitative results of experiments and more detailed theoretical calculations. A comparison

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with the precise experimental data on the magic wavelengths for strontium, ytterbium, and mercury atoms [7, 8] and with the recently measured magic wavelength for magnesium atoms [20] made it possible to refine the rules for choosing the model potential parameters and the algorithm for taking into account the contributions from the inner electrons for numerical estimation of the electromagnetic susceptibilities of atoms [9–11, 21].

An experimental observation of the clock transition of magnesium atoms in a sufficiently strong magnetic field [20] makes it possible to design frequency and time standards based on an optical oscillator with an extremely high  $Q$  factor, controlled by a dc magnetic field. Since the splitting of the  $^3P_{J=0,1,2}$  triplet states of calcium atom exceeds the corresponding splitting in magnesium atoms by a factor of almost 3, it is quite obvious that a stronger magnetic field is necessary for detecting the clock transition line of calcium atoms. To take into account the frequency shift of the clock transition due to the quadratic Zeeman effect and the related uncertainty of the standard clock frequency, one must perform precise measurements of the magnetic field amplitude in the atomic localisation domain.

In this study, we consider the optimal parameters of the optical lattice for magnesium and calcium atoms, which are necessary to minimise the standard clock frequency uncertainties induced by nonlinear and nondipole interactions of atoms with the standing-wave field. The calculations were carried out using previously calculated polarisabilities for clock transitions [11, 21].

Below, unless otherwise specified, we use the atomic system of units, in which  $e = \hbar = m = 1$  and the speed of light  $c$  numerically coincides with the inverse fine-structure constant  $\alpha = 1/137.036$  ( $c = 1/\alpha$ ).

## 2. Energy of atomic vibrational motion in an optical-lattice potential well

The vibrational character of atomic motion in the field of the optical-lattice Stark potential makes the frequencies of the radiation emitted (absorbed) by the lattice-trapped atoms deviate from the frequencies of the radiation emitted by an isolated atom, even when one chooses the magic frequency  $\omega_{\text{mag}}$  for the laser radiation forming the optical lattice [9–11]. This is related to the difference in the spatial distributions of the efficiencies of the dipole (E1) and multipole (M1 and E2) interaction components between the atom and the fields of travelling and standing electromagnetic waves [22, 23]. Therefore, the equality of the shifts of clock transition levels in a travelling wave in no way means their equality in a standing wave. In addition, the equalisation of the polarisabilities determining the intensity-linear Stark effect is insufficient in the field of the atom-trapping optical lattice. Under real conditions, the intensity of the lattice laser field that is necessary to confine atoms is so high that, disregarding the nonlinear effects caused by higher order hyperpolarisabilities, one cannot determine the magic frequency with an accuracy required to compensate completely for the Stark shift of the standard frequency. Along with the difference in the frequency dependences, the hyperpolarisabilities of the clock levels depend differently on the degree of elliptical polarisation of the optical lattice laser radiation [24].

The aforementioned effects lead to the occurrence of additional ‘nonmagic’ uncertainties, related to the difference between the lattice and magic frequencies; these uncertainties

must be compensated for or taken into account when measuring the standard clock frequency with a higher accuracy. To estimate, compensate for, and successfully control the influence of these uncertainties on the measurement accuracy, one can vary the laser field frequency, intensity, and other optical-lattice parameters. In this case, it is necessary to know the details of lattice-induced energy shifts of clock levels with allowance for the nonlinear and nondipole effects of the interaction between an atom and the standing-wave field.

An atom trapped by an optical lattice formed by laser radiation with a frequency  $\omega$  and intensity  $I$  undergoes vibrations in the vicinity of the minimum of Stark potential well. The dependence of the atom-confining potential on the shift  $X$  with respect to the equilibrium position (with allowance for the first nonvanishing anharmonic term) can be written as [9–11]

$$U_{\text{g(e)}}^{\text{latt}}(X, I, \xi) \approx -D_{\text{g(e)}}(I, \xi) + U_{\text{g(e)}}^{\text{harm}}(I, \xi)X^2 - U_{\text{g(e)}}^{\text{anh}}(I, \xi)X^4 + \dots, \quad (1)$$

where

$$D_{\text{g(e)}}(I, \xi) = \alpha_{\text{g(e)}}^{\text{E1}}(\omega)I + \beta_{\text{g(e)}}(\omega, \xi)I^2 \quad (2)$$

is the well depth counted from the minimum energy of free atom; and  $\alpha_{\text{g(e)}}^{\text{E1}}(\omega)$  and  $\beta_{\text{g(e)}}(\omega, \xi)$  are, respectively, the dynamic dipole polarisability and hyperpolarisability of the atom in the ground (g) or excited (e) states. The parameter  $\xi$  determines the degree of circular polarisation of lattice laser radiation, which affects the hyperpolarisability [24]:

$$\beta_{\text{g(e)}}(\omega, \xi) = \beta_{\text{g(e)}}^{\text{lin}}(\omega) + \xi^2[\beta_{\text{g(e)}}^{\text{s}}(\omega) - \beta_{\text{g(e)}}^{\text{lin}}(\omega)]. \quad (3)$$

Here,  $\beta^{\text{lin(c)}}(\omega)$  is the hyperpolarisability in the field of linear (circularly) polarised radiation. The dependence of the atomic oscillation frequency in the potential well (1) on intensity is square-root-like [22, 23]:

$$\Omega_{\text{g(e)}}(I, \xi) = 2\sqrt{E^{\text{rec}}[\alpha_{\text{g(e)}}^{\text{dqm}}(\omega)I + 2\beta_{\text{g(e)}}(\omega, \xi)I^2]}; \quad (4)$$

it is determined by the difference  $\alpha_{\text{c(g)}}^{\text{dqm}}(\omega) = \alpha_{\text{c(g)}}^{\text{E1}}(\omega) - \alpha_{\text{c(g)}}^{\text{qm}}(\omega)$  of the dipole and multipole ( $\alpha_{\text{c(g)}}^{\text{qm}}(\omega) = \alpha_{\text{c(g)}}^{\text{E2}}(\omega) + \alpha_{\text{c(g)}}^{\text{M1}}(\omega)$ ) polarisabilities and by the clock-level hyperpolarisabilities. The relation for frequency (4) can be derived from the expression for the coefficient in the harmonic (quadratic in  $X$ ) term of potential (1):

$$U_{\text{g(e)}}^{\text{harm}}(I, \xi) = [\alpha_{\text{g(e)}}^{\text{dqm}}(\omega)I + 2\beta_{\text{g(e)}}(\omega, \xi)I^2]k^2 = \frac{M\Omega_{\text{g(e)}}^2(I, \xi)}{2}, \quad (5)$$

where  $M$  is the atomic mass and  $k = \omega/c$  is the wave number, which coincides with the momentum of optical lattice photon. In fact, with allowance for the smallness of multipole polarisabilities in comparison with the dipole polarisability ( $|\alpha_{\text{c(g)}}^{\text{qm}}(\omega_{\text{mag}})| \ll |\alpha_{\text{c(g)}}^{\text{E1}}(\omega_{\text{mag}})|$ ), the atomic oscillation frequency (4) is twice the geometric mean of the photon recoil energy  $E^{\text{rec}} = k^2/(2M)$  and the potential depth (2). The expression for the coefficient in the anharmonic term of potential (1)

also depends on the difference between the dipole and multipole polarisabilities and on the hyperpolarisability:

$$U_{g(e)}^{\text{anh}}(I, \xi) = \left[ \alpha_{g(e)}^{\text{dqm}}(\omega) I + 5\beta_{g(e)}(\omega, \xi) I^2 \right] \frac{k^4}{3}. \quad (6)$$

The energy levels of bound vibrational states of atom in potential (1) have the form

$$E_{g(e)}^{\text{vib}}(I, \xi, n) = -D_{g(e)}(I, \xi) + \Omega_{g(e)}(I, \xi) \left( n + \frac{1}{2} \right) - E_{g(e)}^{\text{anh}}(I, \xi) \left( n^2 + n + \frac{1}{2} \right), \quad (7)$$

where  $n = 0, 1, \dots$  is the vibrational quantum number, which can be made minimum ( $n = 0$ ) via additional cooling of lattice-trapped atoms.

When reading the clock transition frequency, the difference in the energies of the initial and final atomic states automatically includes the difference between the vibrational energies (7). As a result, the recorded clock transition frequency acquires an additional shift, which can be written [neglecting the side vibrational frequencies, i.e., on the assumption of invariable vibrational quantum number  $n$  during the atomic transition between clock levels (Lamb–Dicke regime)] as

$$\Delta\nu_{\text{cl}}^{\text{latt}}(I, \xi, n) = E_{\text{e}}^{\text{vib}}(I, \xi, n) - E_{\text{g}}^{\text{vib}}(I, \xi, n) = -\Delta D(I, \xi) + \Delta\Omega(I, \xi) \left( n + \frac{1}{2} \right) - \Delta E^{\text{anh}}(I, \xi) \left( n^2 + n + \frac{1}{2} \right). \quad (8)$$

A specific feature of the anharmonic term of vibrational energy (7) is its linear dependence on intensity:

$$E_{g(e)}^{\text{anh}}(I) = \frac{E^{\text{rec}}}{2} \left[ 1 + \frac{3\beta_{g(e)}(\omega, \xi) I}{\alpha_{g(e)}^{\text{dqm}}(\omega)} \right]. \quad (9)$$

Thus, the anharmonic interaction yields an additional contribution to the term of lattice-induced shift that is linear in  $I$  and proportional to the hyperpolarisability [11]:

$$\Delta E^{\text{anh}}(I) = E_{\text{e}}^{\text{anh}}(I) - E_{\text{g}}^{\text{anh}}(I) = \frac{3E^{\text{rec}}\beta_{g(e)}(\omega, \xi)}{2\alpha_{g(e)}^{\text{dqm}}(\omega)} I. \quad (10)$$

The shift (8) introduces an uncertainty into the measured standard clock frequency, which is related to the nonuniform distribution of the radiation intensity  $\Delta I = I - I_0$  in the localisation domain of lattice-trapped atoms (it is assumed that  $I_0$  is the intensity on the laser beam axis, whereas the intensity distribution in the transverse direction is described by a Gaussian). The deviation  $\delta = \omega - \omega_{\text{mag}}$  of the optical lattice frequency  $\omega$  from the exact value of magic frequency  $\omega_{\text{mag}}$  and the uncertainty of the distribution of vibrational quantum numbers  $n$  over atoms emitting photons with frequency  $\omega$  also contribute to the uncertainty of shift (8). The uncertainty of the distribution of atoms over vibrational states with different  $n$  can be reduced by decreasing the kinetic component of the vibrational energy (7) to the recoil energy  $E^{\text{rec}}$ , which should be lower than the energy of the transition with frequency  $\Omega$  between vibrational levels. To reduce the uncertainties of the standard clock frequency related to those of the laser field intensity and optical lattice frequency, one must perform a detailed analysis of the dependences of shift (8) on  $I$ ,  $\delta$ , and  $\xi$ .

### 3. Determination of the operational magic frequencies of optical lattices for magnesium and calcium atoms

The accuracy of theoretical calculation of the magic frequencies of such many-electron objects as divalent atoms of alkaline-earth like elements is not higher than four or five decimal places. In the long run, the accuracy of determining the magic frequency at a level of eight or nine significant figures is obtained only in precise experimental measurements [7, 8]. One must take into account that the magic frequency providing equality of Stark shifts of atomic clock levels in a travelling wave differs from the magic frequency in a standing wave of the optical lattice [11].

The absence of the intra-atomic magnetic field in bosonic isotopes significantly hinders the observation of the clock transition line and determination of magic frequencies for magnesium and calcium atoms. Obviously, for this reason the magic frequency for magnesium atoms was experimentally measured only accurate to the fifth decimal place [20]. In the case of calcium, only approximate theoretical estimates of  $\omega_{\text{mag}}$  are known to date [11, 15], whose accuracy does not exceed three decimal places. Nevertheless, the up-to-date quantitative estimates of the electromagnetic susceptibilities at magic frequencies make it possible to determine a possible strategy of minimising the nonlinear and nondipole contributions to shift (8) using operational fitting of frequency, polarisation, and intensity of the optical-lattice laser field.

For simplicity, we will consider a one-dimensional lattice and determine the magic frequency by the condition of equality of electric dipole polarisabilities of atoms in the states corresponding to the clock transition levels:

$$\alpha_{\text{e}}^{\text{E1}}(\omega_{\text{mag}}) = \alpha_{\text{e}}^{\text{E1}}(\omega_{\text{mag}}). \quad (11)$$

Having presented shift (8) as a sum of the first few nonvanishing terms in the expansion in powers of intensity  $I$ , which includes root dependences of the difference in the oscillation frequencies  $\Delta\Omega(I, \xi)$  of atom with the same quantum number  $n$  in the lower and upper clock states,

$$\Delta\nu_{\text{cl}}^{\text{latt}}(n, I, \omega, \xi) = c_{1/2}(n, \omega, \xi) I^{1/2} + c_1(n, \omega, \xi) I + c_{3/2}(n, \omega, \xi) I^{3/2} + c_2(\omega, \xi) I^2, \quad (12)$$

we obtain expressions for the coefficients  $c_j(n, \omega, \xi)$  ( $j = 1/2, 1, 3/2, 2$ ) in the form of combinations of the electromagnetic polarisabilities and shift  $\delta = \omega - \omega_{\text{mag}}$ :

$$\begin{aligned} c_{1/2}(n, \omega_{\text{mag}}) &= \left( \frac{\partial \Delta\alpha_{\text{m}}^{\text{E1}}}{\partial \omega} \delta - \Delta\alpha_{\text{m}}^{\text{gm}} \right) \sqrt{\frac{E^{\text{rec}}}{\alpha_{\text{m}}^{\text{E1}}} \left( n + \frac{1}{2} \right)}, \\ c_1(n, \omega_{\text{mag}}, \xi) &= -\frac{\partial \Delta\alpha_{\text{m}}^{\text{E1}}}{\partial \omega} \delta - \frac{3E^{\text{rec}}}{2\alpha_{\text{m}}^{\text{E1}}} \Delta\beta_{\text{m}}(\xi) \left( n^2 + n + \frac{1}{2} \right), \\ c_{3/2}(n, \omega_{\text{mag}}, \xi) &= 2\Delta\beta_{\text{m}}(\xi) \sqrt{\frac{E^{\text{rec}}}{\alpha_{\text{m}}^{\text{E1}}} \left( n + \frac{1}{2} \right)}, \\ c_2(\omega_{\text{mag}}, \xi) &= -\Delta\beta_{\text{m}}(\xi). \end{aligned} \quad (13)$$

Here,  $\Delta\alpha_{\text{m}}^{\text{E1}(\text{qm})}$  and  $\Delta\beta_{\text{m}}$  are the differences in the polarisabilities and hyperpolarisabilities of atoms in the states corresponding to the clock transition levels. The increase in the coefficients  $c_{1/2}$ ,  $c_1$ , and  $c_{3/2}$  with an increase in the vibrational

quantum number indicates that atoms must be retained in the fundamental vibrational state with  $n = 0$ . Therefore, the results of numerical calculations of shift (12) are given below for only the fundamental vibrational state. As follows from (13), when the lattice frequency exactly coincides with the magic frequency ( $\delta = 0$ ) and the multipole and nonlinear effects are neglected ( $\Delta\alpha_m^{\text{qm}} = 0$  and  $\Delta\beta_m = 0$ , respectively), all coefficients  $c_j(n, \omega, \xi)$  turn to zero, as well as shift (12). The multipole effects and lattice frequency shift relative to the magic frequency ( $\delta \neq 0$ ) induce terms with root and linear dependences on  $I$ , although the contribution of hyperpolarisability ( $\Delta\beta_m(\xi) \neq 0$ ) to the linear term is related to the difference in the anharmonic parts of atomic vibrational energy (9), (10) at the upper and lower clock levels. The higher order terms ( $j = 3/2, 2$ ) arise only when the atomic hyperpolarisabilities in the upper and lower clock transition states are taken into account. The atomic polarisabilities in expressions (13) have a subscript  $m$ , which corresponds to the frequency argument of the coefficients in formula (12) equal to the magic frequency ( $\omega = \omega_{\text{mag}}$ ).

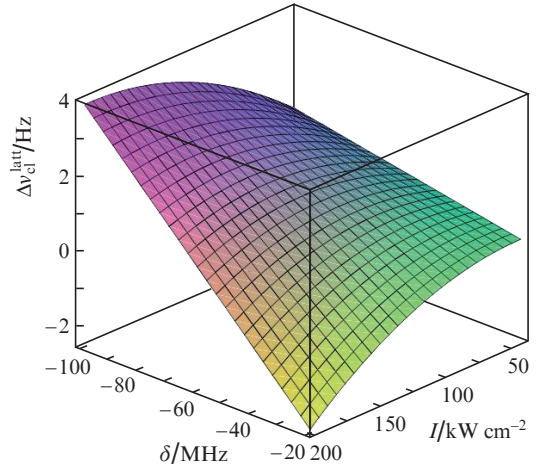
Table 1 contains numerical values of all the quantities entering expression (13); their measurement units suggest that the clock standard frequency shift (12) and laser radiation intensity are expressed in mHz and in  $\text{kW cm}^{-2}$ , respectively. It can be seen that the minimum values of the hyperpolarisabilities of magnesium and calcium atoms correspond to linearly polarised laser radiation of the optical lattice ( $\xi = 0$ ). We choose specifically this case for further numerical calculations. In particular, having expressed  $\delta = \omega - \omega_{\text{mag}}$  in MHz, we arrive at the following expression for magnesium atoms:

$$\begin{aligned} \Delta\nu_{\text{cl}}^{\text{latt}}(n, I, \delta) = & (6.33\delta - 8.25)(n + 1/2)I^{1/2} \\ & - [0.42\delta + (0.397 + 0.021i)(n^2 + n + 1/2)]I \\ & + (0.334 + 0.0177i)(n + 1/2)I^{3/2} - (0.111 + 0.0059i)I^2. \end{aligned} \quad (14)$$

The imaginary part of this shift determines the clock-transition line broadening related to the two-photon ionisation of the upper clock level  $3s3p(^3P_0)$ . The data of Table 1 indicate that at least two bound vibrational states with quantum numbers  $n = 0, 1$  in the optical-lattice potential well may exist only at  $I \geq 20 \text{ kW cm}^{-2}$ . In this case, the binding energy of the fundamental vibrational level with  $n = 0$  is approximately six times higher than the recoil energy  $E^{\text{rec}}$ , and the binding energy of the state with  $n = 1$  almost coincides with  $E^{\text{rec}}$ ; hence, the atom located at this vibrational level becomes free after the first scattering of optical lattice photon. For the fundamental vibrational state at  $I > 20 \text{ kW cm}^{-2}$ , the most important term in expression (14) is that quadratic in  $I$ . Numerical estimates show that, at  $I < 200 \text{ kW cm}^{-2}$ , the corrections to expression (14) that are proportional to higher powers of intensity ( $I^{5/2}, I^3, \dots$ ) do not exceed 0.01% of the

quadratic correction. The negative contribution of the last term on the right-hand side of (14) can be compensated for by only the linear term with a negative  $\delta$  value. Relation (14) can be used to estimate numerically the lattice parameters satisfying the most important conditions for the metrology of magnesium atoms, which require, on the one hand, to hold atoms in the bound states of potential (1), and, on the other hand, to minimise the uncertainties of the clock transition frequency.

Figure 1 shows a dependence of shift (14) on intensity  $I$  and detuning  $\delta$ . Obviously, at a small decrease in the lattice frequency relative to the magic frequency ( $-80 < \delta < -40 \text{ MHz}$ ) and intensities  $I < 100 \text{ kW cm}^{-2}$ , the term linear in  $I$  makes a positive contribution to the shift of standard clock frequency. At sufficiently high intensities ( $I > 100 \text{ kW cm}^{-2}$ ), this contribution is compensated for by the negative quadratic term. Thus, intensity fluctuations in the range of  $90\text{--}110 \text{ kW cm}^{-2}$  barely affect the frequency shift, reducing to minimum the uncertainty of measuring the clock transition frequency. It can be seen in Fig. 1 that the dependence  $\Delta\nu_{\text{cl}}^{\text{latt}}(I)$  is weakest at  $\delta$  values in the vicinity of  $-50 \text{ MHz}$ . In this case, the shift  $\Delta\nu_{\text{cl}}^{\text{latt}}$  is close to zero.



**Figure 1.** Dependence of the frequency shift (14) of the clock transition in magnesium atoms on intensity  $I$  and detuning.

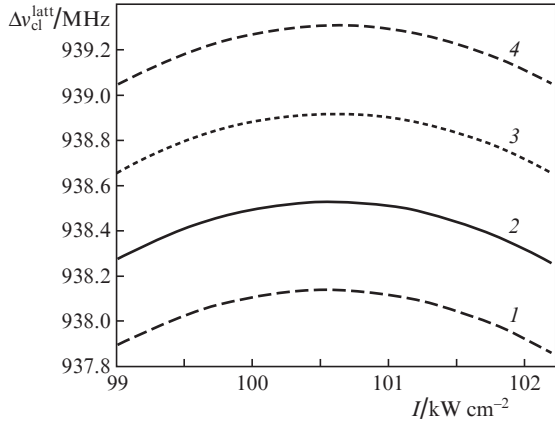
Figure 2 shows the dependences  $\Delta\nu_{\text{cl}}^{\text{latt}}(I)$  for  $\delta = -50 \pm 0.02 \text{ MHz}$ . It can be seen that, for  $\delta = -50 \text{ MHz}$  [curve (3)] and intensity  $I = 100.5 \text{ kW cm}^{-2}$  distributed over different atomic sites in the lattice with a relative uncertainty of  $\pm 1.5\%$ , the shift induced by the lattice field is  $938.7 \pm 0.1 \text{ mHz}$ , which corresponds to an uncertainty of the standard clock frequency of no more than three parts in  $10^{19}$ . At a shift of the lattice frequency with respect to the magic one by  $\delta = -50 \pm 0.2 \text{ MHz}$  and a relative spread of intensity over atomic sites of 10%, the

**Table 1.** Polarisabilities of magnesium and calcium atoms, determining the main parameters of the ‘magic’ lattice, which are necessary to calculate the lattice-induced shifts (12)–(15) and related uncertainties of frequency clock standards.

Atom	$\lambda_{\text{mag}}/\text{nm}$	$\nu_{\text{cl}}/\text{THz}$	$\alpha_m^{\text{E1}}/[\text{kHz}(\text{kW cm}^{-2})^{-1}]$	$\Delta\alpha_m^{\text{qm}}/[\text{mHz}(\text{kW cm}^{-2})^{-1}]$	$\Delta\beta_m^{\text{lin}}/[\mu\text{Hz}(\text{kW cm}^{-2})^{-2}]$	$\Delta\beta_m^{\text{c}}/[\mu\text{Hz}(\text{kW cm}^{-2})^{-2}]$	$\Omega_m/I^{1/2}/[\text{kHz}(\text{kW cm}^{-2})^{-1/2}]$	$\partial(\Delta\alpha_m^{\text{E1}})/\partial\nu/ [10^{-9}(\text{kW cm}^{-2})^{-1}]$	$E^{\text{rec}}/\text{kHz}$	$\nu_0^{\text{BBR}}/\text{GHz}$	$\nu_B/\text{Hz G}^{-2}$
Mg	468.46 [20]	655	17.5	5.48	111 + 5.88i	1735 + 8.69i	51.5	0.42	39.7	0.424	2.173
Ca	747	455	48.0	-2.0	497	1024	41.4	0.273	8.94	0.64	0.8355

Note: the constant  $\nu_0^{\text{BBR}}$  determines the dependence  $\Delta\nu_{\text{cl}}^{\text{BBR}}(T) = -\nu_0^{\text{BBR}}(T/300)^4$  of the thermally induced frequency shift on the environmental temperature  $T$ , and the constant  $\nu_B$  determines the dependence of the quadratic Zeeman frequency shift on the magnetic field;  $\Delta\nu_{\text{cl}}(B) = -\nu_B B^2$ .





**Figure 2.** Dependences of the frequency shift (14) of the clock transition in magnesium atoms on intensity  $I$  at detunings  $\delta = (1) -49.98$ , (2)  $-49.99$ , (3)  $-50.0$ , and (4)  $-50.02$  MHz.

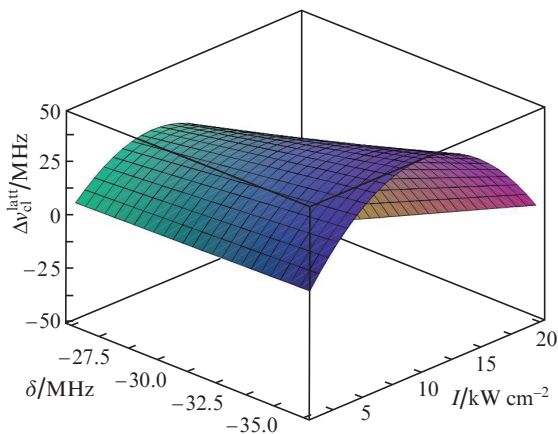
contribution of shift (14) to the uncertainty of the standard clock frequency does not exceed two parts in  $10^{17}$ .

The expression [similar to (14)] for the frequency shift of the clock transition in calcium atoms, induced by a lattice with magic frequency, can be written as

$$\begin{aligned} \Delta\nu_{\text{cl}}^{\text{latt}}(n, I, \delta) = & (0.0589\delta + 0.432)(n + 1/2)I^{1/2} \\ & - [0.273\delta + 0.138(n^2 + n + 1/2)]I \\ & + 0.428(n + 1/2)I^{3/2} - 0.497I^2. \end{aligned} \quad (15)$$

The numerical data of Table 1 show that an intensity of  $I = 10 \text{ kW cm}^{-2}$  is sufficient to trap and confine calcium atoms with four bound vibrational states having vibrational quantum numbers  $n = 0, 1, 2, 3$ . In this case, the well depth  $D$  is more than  $55E^{\text{rec}}$ , the vibrational frequency  $\Omega \approx 15E^{\text{rec}}$ , and the binding energy of the ground state exceeds  $50E^{\text{rec}}$ .

Figure 3 shows a dependence of shift (15) on intensity  $I$  and detuning  $\delta$  for calcium atoms. It can be seen that, at  $\delta = -30$  MHz, the intensity dependence of shift (15) is fairly smooth, so that  $\Delta\nu_{\text{cl}}^{\text{latt}} \approx 34.5$  mHz, with an uncertainty of no more than 1.5 mHz (caused, for example, by a 20% nonuni-



**Figure 3.** Dependence of the frequency shift (15) of the clock transition in calcium atoms on intensity  $I$  and detuning  $\delta$ .

formity of intensity distribution over atomic sites in the optical lattice [ $I = 9 \times (1 \pm 0.2) \text{ kW cm}^{-2}$ ]. This uncertainty corresponds to an uncertainty of standard clock frequency of three to four parts in  $10^{18}$ .

The above calculations demonstrate a number of advantages of calcium atoms in comparison with magnesium ones for precise spectroscopy in optical lattices with magic frequency; these advantages are related to the larger weight of Ca atom and, correspondingly, smaller degree of its ‘heating’ by the recoil energy, and also to its larger electric dipole polarisability, which provides efficient confinement of atoms by the lattice at a laser field intensity of no more than  $10 \text{ kW cm}^{-2}$  (whereas Mg atoms call for an intensity of no less than  $100 \text{ kW cm}^{-2}$ ).

## 4. Conclusions

We performed theoretical calculations and estimations of the frequency shifts of optical clock standards, induced by nonlinear and nondipole effects of interaction of atoms with the field of optical lattice with magic frequency, which yielded quantitative information for precise spectroscopy of ultracold magnesium and calcium atoms in optical lattices. The strongly forbidden transitions between the ground and metastable states of these atoms can be used to develop new frequency standards.

The frequency shifts of the clock transition in magnesium and calcium atoms, induced by the higher order effects of interaction of these atoms with the optical-lattice field, and their dependences on the uncertainty of the frequency and intensity of the laser radiation forming the optical lattice must be taken into account, along with the corrections for the black body radiation (see table), when performing measurements and determining the accuracy of frequency standards. In particular, to reproduce the clock transition frequency in magnesium atoms with a relative uncertainty of no more than  $10^{-17}$ , the operational magic frequency should be 40–60 MHz lower than the magic frequency measured in the weak field of travelling wave and the magnitude of laser frequency deviation from the operational frequency should not exceed 100 kHz. The relative deviation of intensity from the optimal value  $I = 100 \text{ kW cm}^{-2}$ , which is necessary to hold ultracold atoms in the lattice, should not exceed 10%–15%.

The similar decrease in the operational lattice frequency for calcium atoms by 29–30 MHz in comparison with the magic frequency makes it possible to reduce the frequency standard uncertainty induced by nonlinear, nondipole, and anharmonic effects of interaction of Ca atoms with the optical-lattice field. In particular, a frequency standard uncertainty at a level of three to four parts in  $10^{18}$  can be attained at a relative uncertainty of laser frequency in the tenth decimal place and at a 20% nonuniformity of intensity distribution over atomic sites in the lattice. Since calcium atoms have a higher (by a factor of almost 3) electric dipole polarisability and lower recoil energy as compared with magnesium, the optimal intensity of lattice laser radiation can be almost an order of magnitude lower than that for Mg atoms.

Bosonic atoms with zero nuclear magnetic moments dominate in natural magnesium and calcium isotopes. This circumstance calls for fairly strong magnetic fields in order to induce and detect strongly forbidden radiative transitions between the clock energy levels in these elements. Estimations of the probability of the magnetically induced decay of a metastable state show that one must use magnetic fields

higher than 100 G for stable observation of a clock transition. The clock transition frequency changes due to the quadratic Zeeman effect by more than 20 and 8 kHz in Mg and Ca atoms, respectively. At an uncertainty of the acting magnetic field at a level of seventh decimal place, the Zeeman shift introduces an uncertainty into the standard clock frequency at a level of a few parts in  $10^{17}$ .

The results of numerical calculations of electromagnetic polarisabilities, given in the table, were obtained based on the modified model potential method, whose error can be estimated as 5%–7% [11].

The data obtained are indicative of significant differences in the possibilities of practical manipulation with magnesium and calcium atoms in optical lattices. In particular, the uncertainty of the clock standard frequency shift related to the non-uniform distribution of radiation intensity in the direction perpendicular to the laser beam for calcium atoms is much smaller than that for magnesium atoms, as follows from comparison of Fig. 3 with Figs 1 and 2.

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