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Magic Wavelengths of the Optical Clock Transition at 1107 nm of Barium *

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Magic wavelengths for laser trapping of barium atoms in the optical lattices are calculated with considering the optical clock transition at 1107 nm between the $6s^2\ {}^1S_0$ state and $6s5d\ {}^3D_1$ state. Theoretical calculation shows that there are several magic wavelengths with the linearly polarized trapping laser. The trap depths of the optical lattice and the slope of light shift difference with different magic wavelengths are also calculated. Some of these magic wavelengths are selected and recommended as potentially suitable magic wavelengths for the optical lattice trapping laser.

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Recent progress in the manipulation of cold or ultracold neutral atoms offers advancement in a wide variety of applications. Possible applications include the optical lattice clock,[1−3] which may attain relative uncertainty of 10^{-18}, more accurate measurements of fundamental constants,[4,5] enabling new tests of fundamental physics,[6−9] establishing the new quantum computational schemes[10,11] and so on. In a far-detuned optical dipole trap, the atoms are tightly localized so that Doppler and photon-recoil related effects on the transition frequency are eliminated.[12,13] Meanwhile, the wavelength of the trapping laser is carefully chosen (called magic wavelength) so that the ac Stark shift has essentially no effect on the internal clock transition frequency, i.e., the ac Stark shift potentials of the clock transition levels are equal to each other and the differential light shift is canceled. This optical lattice approach combines the advantages of ions and neutral atoms in frequency standards by using large particle numbers and a confining optical potential, which can greatly improve the established high-accuracy frequency standards based on neutral atoms. The frequency standards of Sr and Yb atoms based on optical lattice traps have achieved great successes.[1,2,14−16] Some progress has also been made in the cold Hg atom,[17,18] which seems to be the most promising candidate for the optical lattice clocks in the long run. In the past few years, the cesium primary frequency standard with atoms trapped in an optical lattice with a magic wavelength was suggested,[19,20] different optical clock schemes based on cold atoms trapped with the magic wavelength lasers had been proposed and the possible magic wavelengths for the optical clock transitions in aluminium, gallium, dysprosium and barium atoms were also calculated.[21−24] The teraherz clocks based on optical lattices trapped cold Mg, Ca and Sr atoms have also been proposed[25] in recent years.

In contrast to the continuously increasing interest in the optical clocks with the trapped alkaline-earth metal Sr atoms and rare-earth metal Yb atoms, and the microwave frequency standard with cold cesium atoms, in this Letter we investigate the potential optical clock with the alkaline-earth metal Ba atoms in an optical lattice, focusing on the wavelength-dependent ac Stark shifts caused by the trapping laser for the optical clock transitions. Barium is also a good candidate for the optical clock. The laser cooling and trapping of Ba atoms was reported[26] in 2009, and the minimum achieved temperature of the trapped barium cloud is about 5.7(8) mK[27] in the magneto-optical trap. There are three electric quadrupole (E2) transitions[28,29] in barium lines from the ground state $6s^2\ {}^1S_0$ to the metastable states $6s5d\ {}^3D_2$ at 1085 nm, $6s5d\ {}^3D_1$ at 1107 nm and $6s5d\ {}^1D_2$ at 877 nm. The state ${}^3D_2$ has a lifetime of about 69 s and the state ${}^1D_2$ has a lifetime of about 0.5 s. Although the exact lifetime of the metastable state ${}^3D_1$ is not determined, the lifetime of the ${}^3D_1$ state[26,30] is evaluated about tens of seconds and even longer than the state ${}^3D_2$. The natural linewidths of these three E2 transitions are very sharp so that these E2 transitions of barium could be used for the optical frequency standard. In addition, barium is also heavy, which helps to contain the motional effects. In the previous works,[23,24] we presented the calculations of the magic wavelengths for the $6s^2\ {}^1S_0$–$6s5d\ {}^3D_2$ clock transition at 1085 nm and the $6s^2\ {}^1S_0$–$6s5d\ {}^1D_2$ clock transition at 877 nm. In the present study, we evaluate the ac Stark shifts and magic wavelengths for another optical clock tran-

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sition $^1S_0$–$^3D_1$ at 1107 nm. This clock transition has a natural width of ≈1 mHz, which is narrower than the natural widths of the clock transitions at 1085 nm (≈2 mHz) and 887 nm (≈0.3 Hz), and it seems to be able to compete for the next-generation frequency standard with the Sr atoms clock transition with a natural width of ≈1 mHz[31] and the Yb atoms clock transition with a natural width of ≈10 mHz.[32] The theoretical calculation about the lifetime and natural linewidth of the state $^3D_1$ will be carried out in the subsequent study. Some other effects such as the black-body radiation (BBR) shift of the proposed optical clock transitions and the collisional properties of barium atoms will be discussed elsewhere.

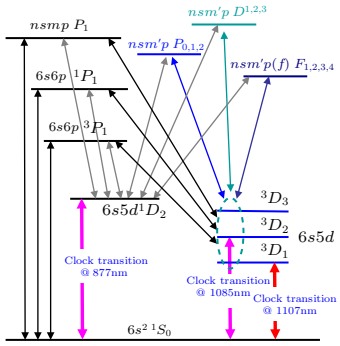


Fig. 1. Simplified diagram of the energy levels for Ba atoms with some possible laser couplings. The metastable triplet states $6s5d\ ^3D_J$ ($J = 1, 2, 3$) are signed by the oval, and the optical clock transitions at 887 nm, 1085 nm and 1107 nm are also marked.

Table 1. Atomic transition data of the $^1S_0$ and $^3D_1$ states of Ba: energy level, wave number (WN) (cm^{-1}), Einstein coefficients between the states $|k\rangle$ and $|i\rangle$, i.e. A_{ik} ($10^6 s^{-1}$).

Lower state $\|i\rangle$	Upper state $\|k\rangle$	WN (cm^{-1})	A_{ik} ($10^6 s^{-1}$)	References
$6s5d\ ^3D_1$ 9033.966 cm^{-1}	$6s7p\ ^1P_1$	32547.033	0.15	Ref. [40]
	$6s7p\ ^3P_2$	30987.240	0.121	Ref. [39]
	$6s7p\ ^3P_1$	30815.512	2.65	Ref. [39]
	$6s7p\ ^3P_0$	30743.490	9.87	Ref. [39]
	$5d6p\ ^3P_2$	25956.519	14	Ref. [39]
	$5d6p\ ^3P_1$	25704.110	28	Ref. [37]
	$5d6p\ ^3P_0$	25642.126	80	Ref. [37]
	$5d6p\ ^3D_2$	24531.513	11.0	Ref. [37,40]
	$5d6p\ ^3D_1$	24192.033	38.0	Ref. [37]
	$5d6p\ ^1D_2$	23074.387	11	Refs. [37,38]
	$5d6p\ ^3F_2$	22064.645	15.2	Refs. [37,38]
	$6s6p\ ^1P_1$	18060.261	0.0031	Ref. [37]
	$6s6p\ ^3P_2$	13514.745	0.01003	Ref. [39]
	$6s6p\ ^3P_1$	12636.623	0.1267	Ref. [39]
	$6s6p\ ^3P_0$	12266.024	0.35	Ref. [39]
$6s^2\ ^1S_0$ 0 cm^{-1} (ground state)	$6s18p\ ^1P_1$	41 494.39	0.086	Ref. [37]
	$6s17p\ ^1P_1$	41411.04	0.15	Ref. [37]
	$6s16p\ ^1P_1$	41307.88	0.23	Ref. [37]
	$6s15p\ ^1P_1$	41183.60	0.56	Ref. [37]
	$5d8p\ ^3P_1$	41097.20	0.72	Ref. [37]
	$6s14p\ ^1P_1$	40991.23	0.14	Ref. [37]
	$5d8p\ ^3D_1$	40893.76	0.45	Ref. [37]
	$6s13p\ ^1P_1$	40765.23	0.081	Ref. [37]
	$6s12p\ ^1P_1$	40428.68	0.46	Ref. [37]
	$6s11p\ ^1P_1$	39982.14	1.5	Ref. [37]
	$6s10p\ ^1P_1$	39311.95	0.041	Ref. [37]
	$6s9p\ ^1P_1$	37775.28	1.1	Ref. [37]
	$6s7p\ ^1P_1$	32547.033	42.0	Ref. [37]
	$6s7p\ ^3P_1$	30815.512	0.013	Ref. [39]
	$5d6p\ ^1P_1$	28554.221	35.0	Ref. [37]
	$5d6p\ ^3P_1$	25704.110	1.1	Ref. [37]
	$5d6p\ ^3D_1$	24192.033	1.50	Refs. [37,38]
	$6s6p\ ^1P_1$	18060.261	119	Refs. [37,38]
	$6s6p\ ^3P_1$	12636.623	0.299	Ref. [41]

For alkaline-earth metal Ba atoms, two valence electrons result in two series of atomic energy levels as the electron spins can be parallel (triplet states) or anti parallel (singlet state). The lowest metastable states $6s5d\ ^3D_J$ could be divided into three fine structure sublevels $^3D_3$, $^3D_2$ and $^3D_1$. For the ^3D_J and $^1D_2$ metastable states, the transitions to higher states can be mainly divided into three groups: D_J–$P_{J'}$, D_J–$D_{J'}$, and D_J–$F_{J'}$. The energy diagram can be simplified as shown in Fig. 1 and the levels in the oval are the metastable states $6s5d\ ^3D_J$ states. The optical clock transitions at 877 nm, 1085 nm and 1107 nm are also marked in Fig. 1.

We focus on the optical clock transition from $6s^2$

$^1S_0$ to $6s5d\ ^3D_1$ and calculate the ac Stark shifts of the magnetic sub levels. The magic wavelength for trapping Ba atoms in an optical lattice could be obtained by matching the ac polarizabilities of the atomic $^1S_0$ and $^3D_1$ magnetic sub levels. There are two sets of formulas to calculate the atomic ac polarizability, both of them are derived from the second-order perturbation theory and could lead to the same results. One method is to regard the total ac polarizability of the atomic state as composed by two parts:[33] the scalar polarizability α_0 and the tensor polarizability α_2. Here we choose another set of formulas to carry out our calculation, following Refs. [34–36]. Using the second-order perturbation theory, the energy shift $U_i(\omega, p, m_i)$ caused by the trapping laser field for the Zeeman sublevel m_i of the atomic state $|i\rangle$ with energy E_i can be expressed with the induced polarizability $\alpha_i(\omega, p, m_i)$ as follows:

$$U_i(\omega, p, m_i) = -\alpha_i(\omega, p, m_i) I/2\varepsilon_0 c, \tag{1}$$

where I is the laser intensity, p is the laser polarization, ε_0 is the dielectric constant and c is the speed of light in a vacuum. The frequency of the trapping laser $v = \omega/2\pi$. The induced polarizability $\alpha_i(\omega, p, m_i)$ can be calculated by summing up the contributions from all dipole transitions from the fine structure level i to all other fine structure levels k with the respective Einstein coefficients A_{ki} and Zeeman sublevels m',

$$\alpha_i = 6\pi c^3 \varepsilon_0 \sum_{k,m'} \frac{A_{ki}(2J_k+1)}{\omega_{ik}^2(\omega_{ik}^2 - \omega^2)} \begin{pmatrix} J_i & 1 & J_k \\ m_i & p & -m' \end{pmatrix}^2, \tag{2}$$

where the transition frequencies $v_{ik} = \omega_{ik}/2\pi = (E_k - E_i)/h$, assuming the level energy $E_k > E_i$, the expression in large parentheses denotes a $3J$ symbol, which describes the selection rules and relative strength of the transition depending on the involved angular momenta J, the projection m, and the polarization p. We can obtain the polarizability α_i if we know the data of ω_{ik} and A_{ki} in Eq. (2).

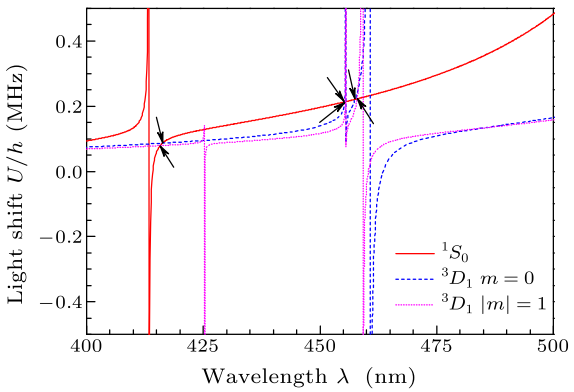


Fig. 2. The wavelength dependence of the light shifts of the $^1S_0$ and $^3D_2(m = 0, \pm 1)$ sub levels on a linearly polarized trapping laser wavelength from 400 nm to 500 nm.

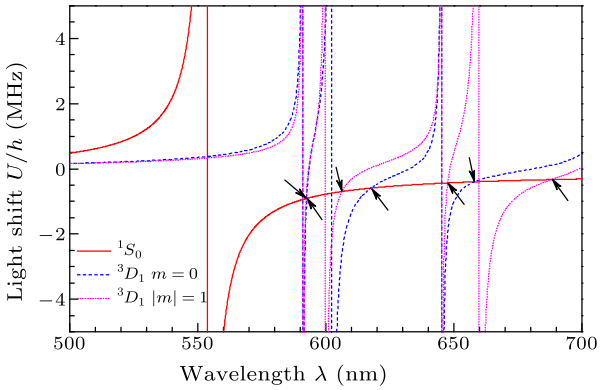


Fig. 3. The wavelength dependence of the light shifts of the $^1S_0$ and $^3D_2(m = 0, \pm 1)$ sub levels on a linearly polarized trapping laser wavelength from 500 nm to 700 nm.

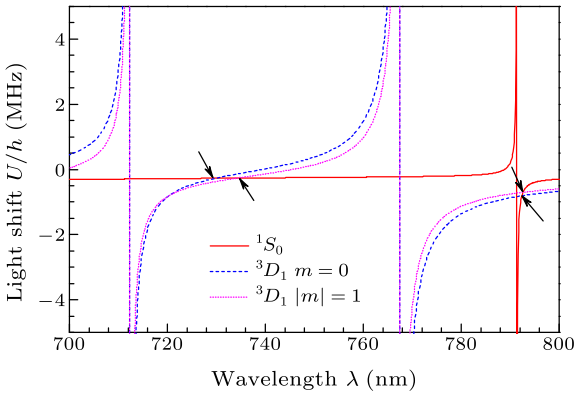


Fig. 4. The wavelength dependence of the light shifts of the $^1S_0$ and $^3D_2(m = 0, \pm 1)$ sub levels on a linearly polarized trapping laser wavelength from 700 nm to 800 nm.

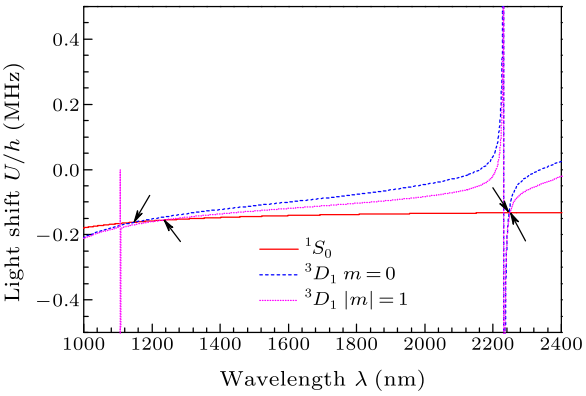


Fig. 5. The wavelength dependence of the light shifts of the $^1S_0$ and $^3D_2(m = 0, \pm 1)$ sub levels on a linearly polarized trapping laser wavelength from 1000 nm to 2400 nm.

We choose the boson isotope ^{138}Ba with the nuclear spin $I = 0$, thus we can carry out the calculations without considering the hyperfine structure. The magnetic field is set to be zero and the trapping light is assumed to be linearly polarized so that the effects of the magnetic field could be left out of the account during our calculations.

The atomic transition data including level energy wave numbers (WN) and probabilities (Einstein coefficients A_{ki}) of the ground state $^1S_0$ and the metastable

triplet state $^3D_1$ of Ba atoms are listed in Table 1. The available experimental values are selected as much as possible mainly from Refs. [37,38], and for the rest we mostly take part of the theoretical and experimental data from Refs. [39–41]. The ionization limit atomic level of barium is 42034.91 cm^{-1} and the effects of highly excited states and continuum states are ignored due to the fact that these effects would only make a slight contribution to the atomic ac polarizabilities as considered in this work.

Using the method described above and the data in Table 1, the polarizabilities and light shifts of the atomic states $^1S_0$ and $^3D_1$ of Ba atoms could be calculated, and the magic wavelengths for the optical clock transition could then be obtained.

The dependence of the induced light shifts for the metastable state $6s5d\ ^3D_1$ ($m = 0, \pm 1$) sub levels and the ground state $6s^2\ ^1S_0$ on the wavelength λ of a linearly polarized trapping laser is illustrated in Figs. 2–5. Our calculation is carried out under the condition that the trapping laser intensity is 10^4 W/cm^2 and the longitudinal axis represents the induced light shift in units of MHz. The magic wavelengths take place when the induced light shifts of the optical clock transition levels equal to each other, as marked by the arrows. The wavelength range of the trapping laser in our calculation is from 400 nm to 3000 nm and there are 21 magic wavelengths altogether, as listed in Table 2.

The trap depth of the optical lattice is defined as the maximum temperature of the trapped atoms $T = |U|/k_B$, where U is the ac Stark shift potential (the light shift) and k_B is the Boltzmann constant. We have calculated the trap depths of the optical lattice using the linearly polarized laser with the different magic wavelengths, assuming the laser intensity to be 10^4 W/cm^2. The trap depths would help us to choose the suitable working points.

The slope of light shift difference with the given magic wavelength, which is defined as $k = \frac{d}{d\lambda}(\Delta U)$ and shows how fast the difference changes with the laser wavelength perturbations, has also been considered. Here $\Delta U = |U_j - U_i|$ is the difference of the light shifts for the atomic sub level j and i. In terms of the barium optical clock transition considered in this work, $\Delta U = |U_{^3D_1} - U_{^1S_0}|$. A strong slope will lead to a zero crossing for the differential polarizability and should be avoided in the optical lattice clock experiments. The slopes of light shift difference with different magic wavelengths are calculated assuming that the laser intensity is also 10^4 W/cm^2.

Table 2. The ac Stark shift potentials, trap depths and the light shift slopes of the optical lattice with different magic wavelengths. The relevant data are obtained under the condition that the trapping laser intensity is 10^4 W/cm^2.

Magic wavelength (nm)	Corresponding clock transition	ac Stark shift potential (MHz)	Trap depth (μK)	Slope (Hz/GHz)
415.8	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	0.0790	3.8	9.58
416.3	$^1S_0 \rightarrow {}^3D_1$ (m=0)	0.0866	4.2	6.78
455.3	$^1S_0 \rightarrow {}^3D_1$ (m=0)	0.2133	10.2	163.54
455.4	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	0.2137	10.3	2853.52
457.5	$^1S_0 \rightarrow {}^3D_1$ (m=0)	0.2210	10.6	24.38
457.9	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	0.2224	10.7	65.39
592.3	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.9125	43.8	1687.68
592.5	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.9079	43.6	1732.81
606.3	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.6961	33.4	171.64
617.6	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.5900	28.3	61.64
647.6	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.4326	20.8	916.49
658.1	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.3985	19.1	43.23
688.1	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.3304	15.9	8.27
729.7	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.2718	13.0	56.89
734.3	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.2665	12.8	38.73
792.4	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.7960	38.2	1081.56
792.6	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.7061	33.9	758.69
1150.8	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.1615	7.8	0.58
1228.7	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.1558	7.5	0.34
2246.8	$^1S_0 \rightarrow {}^3D_1$ (m=0)	−0.13284	6.4	113.66
2249.6	$^1S_0 \rightarrow {}^3D_1$ ($\|m\|$=1)	−0.13282	6.4	77.78

The calculation results of the ac Stark shift potentials, trap depths and light shift slopes with different magic wavelengths are listed in Table 2. The unit for the slopes of light shift difference with the given magic wavelength k has been converted from MHz/nm to Hz/GHz via $|d(\Delta U)/d\upsilon| = |(\lambda^2/c) \times [d(\Delta U)/d\lambda]|$, where λ is the magic wavelength.

When selecting magic wavelengths for the optical lattice, the trap depths should be deep enough to trap atoms and meanwhile the slopes of light shift difference should be small. In general, the slopes would be less than 100 Hz/GHz. Another consideration is the accessibility of the magic wavelengths. The temperature of the atoms trapped in the optical lattice is commonly about several μK,[42,43] therefore, we could select several magic wavelengths potentially

suitable for the optical lattice trapping laser according to our calculation results listed in Table 2. The potentially magic wavelengths are 457.5 nm, 457.9 nm, 617.6 nm, 658.1 nm, 688.1 nm, 729.7 nm, 734.3 nm, 1150.8 nm and 1228.7 nm, respectively, due to the fact that the shift slopes are a lot smaller compared with the other magic wavelengths and the trap depths with these magic wavelengths could also be deep enough for trapping atoms due to the availability of current lasers. Benefiting from the development of the laser technology and the laser frequency stabilization technique, the high power amplified diode lasers with narrow linewidth (laser intensity reaches the magnitude of 10^4 W/cm^2, line width is commonly less than 1 kHz) could be achieved in the wavelength range from about 400 nm to 1800 nm.

In summary, we have calculated the wavelength-dependent ac Stark shifts of the optical clock transitions from $6s^2\ {}^1S_0$ to $6s5d\ {}^3D_1$ with all the magnetic sub levels of barium atoms, and have obtained the magic wavelengths for the optical lattice trapping laser. The trap depths and light shift slopes for the optical lattice traps with different magic wavelengths have also been evaluated. According to our calculations and discussions, we select 457.5 nm, 457.9 nm, 617.6 nm, 658.1 nm, 688.1 nm, 729.7 nm, 734.3 nm, 1150.8 nm and 1228.7 nm as potentially suitable magic wavelengths for the optical lattice trapping laser. Our calculations are carried out without considering the effects of the magnetic field although there is always a residual magnetic field for an operational clock. It would be a long way to build an accurate optical clock with cold barium atoms trapped in the optical lattice, and our results should be useful for giving impetus to the study of the optical frequency reference based on barium atoms.

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