

SPECTROSCOPIC CHARACTERISTICS OF ALKALINE-EARTH ATOMS FOR ATOMIC FREQUENCY STANDARDS

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ABSTRACT

A brief overview concerning the motivations and the precise calculations for the spectroscopic characteristics of alkaline-earth atoms is given. In particular, the effect of hyperfine-induced singlet-triplet mixing on radiative lifetimes and light shift have been studied in neutral strontium.

1. INTRODUCTION

Alkaline-earth atoms are widely used in a number of important applications including atomic clocks, laser cooling of atoms at temperatures close to the recoil limit, parity-nonconserving experiments, the search for a permanent electron dipole moment, atomic interferometry, etc. Presently, there is also important interest in properties of divalent atoms in conjunction with low-temperature Bose-Einstein condensation experiments [1].

This paper is motivated by emerging experiments on cooling and trapping of alkaline-earth atoms [2], in particular, on sideband cooling and spectroscopy neutral atoms in the Lamb-Dicke confinement [3,4].

In the first part of the paper, we estimate theoretically the single-photon decay channel from the lowest-energy 3P_0 state of alkaline-earth atoms. By consideration of the prospects for an optical clock on the $J=0 \leftrightarrow J'=0$ transition, it was shown, that hyperfine structure (hfs) effects can mix significantly levels which cross for some atomic isotopes with nonzero nuclear spin ($I \neq 0$). In particular, in the case of ^{87}Sr atoms, the hfs mixing of the 3P_0 ($I=9/2$) state with the $^{1,3}P_1$ states give rise to an electric-dipole transition rate. In the present calculations the non-relativistic Hamiltonian of hfs-interaction including the dipole contact interaction, the magnetic dipole orbital interaction, the magnetic spin-dipolar interaction and electric quadrupole interaction, is used.

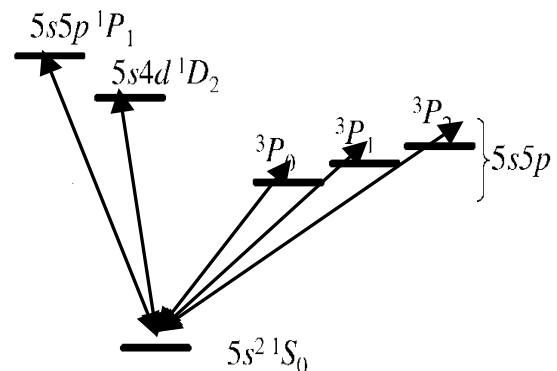
The second part contains the precise theoretical results for the a.c. Stark shift on fine-structure components of ^{87}Sr atoms both in the ground $5s^2\ ^1S_0$ and $5s5p\ ^3P_0$ excited state on the framework of the measurements with the Lamb-Dicke confinement of neutral atoms [3,4]. For that purpose we introduce few separate differential susceptibilities (polarizabilities and hyperpolarizabilities) to describe of the calculating approaches based on the Green's function method in the framework of the model potential approximation and on the multiconfiguration Dirac-Fock self-

consistent field program [5]. Here we report our results for the light shift as a function of the laser wavelength and polarization.

2. HFS-INDUCED DECAY RATE FOR $5s5p\ ^3P_0$ - STATE OF ^{87}Sr

As the prime candidates for an optical frequency standard in alkaline-earth atoms are the long-lived spin-forbidden transitions. Recently, H.Katori et al [3] reported on a narrow-line laser cooling and trapping of ^{87}Sr atoms by employing a magneto-optical trap (MOT) on the $5s5p\ ^3P_1 - 5s^2\ ^1S_0$ transition at 689 nm (Figure.1). They have received laser-cooled an atomic sample down to the photon recoil temperature of 400 nK with a phase space density about of 10^{-2} .

Figure 1. Schematic energy-level diagram for neutral strontium.



The metastable $5s5p\ ^3P_2$ - and $5s4d\ ^1D_2$ -states can also serve as an effective ground state in such experiments [6].

As usually, the natural radiative lifetimes do not normally show any dependence of the hfs-quantum number F within a state considered, since the lifetime is mainly an electronic quantity. On a framework of such assumption, the $J=0 \leftrightarrow J'=0$ transitions (Figure 1) are strongly forbidden by the rigorous selection. Nevertheless, there can be such hfs-dependence due to hfs-induced mixing between levels with different radiative lifetimes. In that case the hfs-interaction can mix significantly levels which cross for some specific nuclear charge for isotopes with nonzero nuclear spin ($I \neq 0$).

Early observations of forbidden transitions that were later identified as nuclear-spin-induced absorption lines

such as $^1S_0 - ^3P_2$ [7] and $^1S_0 - ^3P_0$ [8] in Hg I. Extensive calculations of the nuclear-spin-induced transition rates were made by Garstang [9].

Two approaches have been used to treat the radiative decay of hfs-levels. The first is the perturbative approach in which the hfs-levels are determinate by diagonalizing the hfs-energy matrix [10]. This approach is appropriate for cases such as the $J=0 \leftrightarrow J'=0$ transition, where the radiative linewidths of the levels are small compared to the levels spacing. In the second approach the radiative field and the hfs-interaction are treated together.

In the present paper such hfs-effects for the $5s5p\ ^3P_0 - 5s^2\ ^1S_0$ transition in the strontium atoms are considered for the first time. It is important to note, that the hfs-effect can only exist in the ^{87}Sr isotope ($I=9/2$), since it is the only stable one having a nonzero nuclear magnetic moment.

A sketch of the theory applied is as follows: The expression for the perturbed wave function becomes

$$| ^3P_0, FM \rangle_1 = | ^3P_0, FM \rangle - \int H_{hfs} G | ^3P_0, FM \rangle$$

Here zero-order states $| ^3P_0, FM \rangle$ are sums of products of electron eigenstates and nuclear spin functions, combined to give total angular momentum F with z -component M , G is the reduced Green's function with an energy $E(^3P_0)$, H_{hfs} is the hfs-Hamiltonian. The first-order perturbed wave function for the 3P_0 -state is given by

$$\begin{aligned} | ^3P_0, FM \rangle_1 &= | ^3P_0, FM \rangle \\ &+ \frac{\langle ^3P_1, FM | H_{hfs} | ^3P_0, FM \rangle}{E(^3P_0) - E(^3P_1)} | ^3P_1, FM \rangle \\ &+ \frac{\langle ^1P_1, FM | H_{hfs} | ^3P_0, FM \rangle}{E(^3P_0) - E(^1P_1)} | ^1P_1, FM \rangle, \end{aligned}$$

where mixing with only lowest 3P_1 and 1P_1 states by the nuclear perturbation is included. The wave functions $^{1,3}P_1$ can be written approximately as linear combinations of the unperturbed wave functions $^{1,3}P_1^0$ in a purely LS-coupled scheme.

Finally, the decay rate for a dipole transition from the excited 3P_0 state to the ground 1S_0 state is

$$A_{hfs}(^3P_0) = \frac{4\alpha \omega^3}{3 c^2} \sum_{M'} \langle S_{FM'FM} \rangle,$$

where ω is the transition frequency and

$$S_{FM'FM} = \langle ^1S_0, FM' | r_1 + r_2 | ^3P_0, FM \rangle_1.$$

The calculated decay rate in ^{87}Sr atom for the $5s5p\ ^3P_0$ state with $F=I=9/2$ is $1/183\text{ s}^{-1}$. The calculations are carried out using multiconfiguration Dirac-Fock program code (GRASP package code[5]) and corresponding values for the hfs-contributions from [11].

Thus, this result can be considered as an unique possibility for applications in the optical clocks because of its narrow line found in the hfs-induced $5s5p\ ^3P_0 - 5s^2\ ^1S_0$ transition in the strontium atoms.

3. LIGHT SHIFT FOR ^{87}Sr OPTICAL CLOCK ON THE $5s5p\ ^3P_0 - 5s^2\ ^1S_0$ TRANSITION

Shift ΔE and splitting of energy levels induced by the laser with a frequency ω are determined by the roots of the secular equation

$$\det \|\Delta E \delta_{M'M} - V_{M'M}\| = 0.$$

Here $V_{M'M}$ is the matrix element of the atom-field interaction operator

$$\begin{aligned} U(\vec{r}, t) &= v(\vec{r}) e^{-i\omega t} + v^+(\vec{r}) e^{i\omega t}, \\ v(\vec{r}) &= -\frac{1}{2} \vec{E}(\vec{e} \cdot \vec{D}), \end{aligned}$$

associated with the action of monochromatic radiation with electric-field strength

$$\vec{E}(\vec{r}, t) = \vec{E} \text{Re} \{ \vec{e} \exp[i(\vec{k} \cdot \vec{r} - \omega t)] \}.$$

Here \vec{e} is the unit polarization vector and \vec{k} is the wave vector, \vec{D} is the atomic dipole moment.

It is convenient to express the general formula for $V_{M'M}$ as the sum of the second-order and fourth-order matrix elements by using well known terms of the perturbation theory

$$V_{M'M} = V_{M'M}^{(2)} + V_{M'M}^{(4)},$$

where

$$\begin{aligned} V_{M'M}^{(2)} &= -\langle nJM | UGU | nJM' \rangle, \\ V_{M'M}^{(4)} &= -\langle nJM | UGUGUGU | nJM' \rangle \\ &+ \langle nJM | UGU | nJM' \rangle \langle nJM | UGGU | nJM' \rangle \end{aligned}$$

and

$$\leftrightarrow = \sum_{\Delta P} \frac{\left| \langle P \Delta \rangle \langle P \Delta \rangle \right|}{E_{P \Delta} - E_a}$$

is the quasi-energy Green's function of the atom and $E_{n\kappa} = E_n + \kappa\omega$ is the quasi-energy; the double brackets here mean the integration over the spatial variables of the atom and averaging over the time in the matrix elements. The first term for V_{MM} in the field expansion can be interpreted as the a.c. polarizability (α) which has the scalar and tensor parts [12-14] and the next terms correspond to the a.c. hyperpolarizability (γ) of the state considered.

After the time averaging and angular integration, applying angular momentum theory allows the a.c. susceptibilities to be resolved into irreducible parts [12-14]. For example, the fourth-order term in the field with linear polarization is determined by only three invariant atomic parameters, which correspond to the scalar part of hyperpolarizability, and to two tensor parts having rank 2 and 4, respectively. However, for the circular polarization of the electromagnetic wave, the non-zero fourth-order correction is determined by five invariant atomic parameters (one scalar part, one asymmetric (vector) part and three tensor (symmetric) parts).

Thus, in the presence of the external laser field the observed transition frequency is written as

$$\nu = \nu^{FM} - \Delta\alpha\omega\hbar\tilde{M}d^s - \frac{A}{EG}\Delta\gamma\omega\hbar\tilde{M}d^E - \hbar\hbar\hbar F$$

where $\hbar\nu^{(0)}$ is the transition energy for the unperturbed atomic states. Evidently, that the level of the experimental accuracy can be increased significantly by using any specific trapping laser frequency ω and the type of polarization vector; all that can provide exact cancellation of the second-order terms (a.c. polarizabilities).

In the view of the situation presented above, the goal of this section is a theoretical analysis of the field-induced terms up to the order of F^4 as the function of the laser frequency and polarization.

Accurate calculations of the matrix elements for the components of the susceptibilities require reliable wavefunctions which should give correct values for both of the quantities. In the present paper we used multiconfiguration Dirac-Fock (GRASP [5]) program for that purpose. The key point is that it is consistent to use precise wave functions for the evaluation of dipole matrix elements, together with experimental transition energy. To control results we have also carried out similar calculations with the Fues' model potential method [12]. Quite simple analytical presentation for the Green's function enables us to evaluate the contribution of the higher excited states (including continuum) which are neglected in the finite-sum approach.

Results of our calculation are shown on Figure 2 as a function of the laser wavelength.

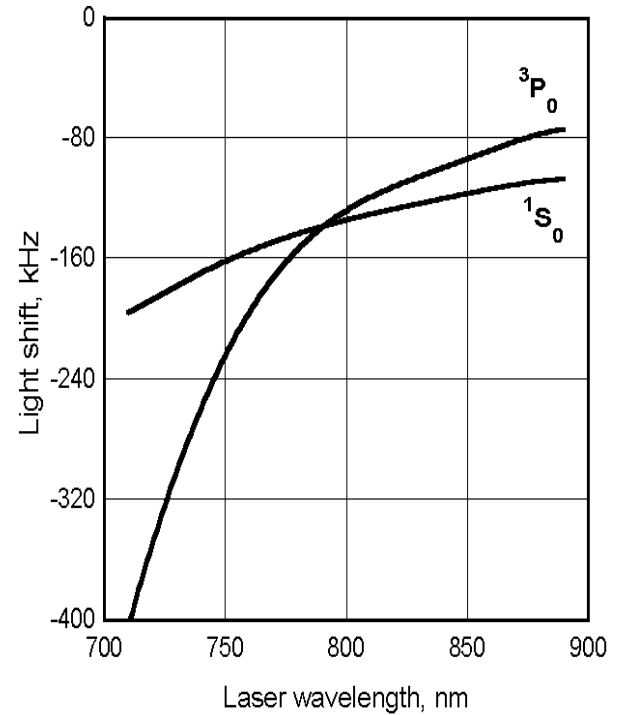


Figure 2. Light shift as a function of the trapping laser wavelength at intensity $100 \text{ mW}/\pi(17\mu\text{m})^2$ in the vicinity of the crossed point. Linearly polarized beam is used.

The crossing point for the both $5s5p \ ^3P_0$ and $5s^2 \ ^1S_0$ states is realised at the wavelength of about 790 nm. In order to evaluate this point, we note that fourth-order Stark contribution is not large enough to be significant employing trapping laser intensity presented above.

3. CONCLUSION

In connection with laser cooling spectroscopy measurements which have been carried out and planned [3,4], we have investigated the light shift for the hfs-induced $5s5p \ ^3P_0 - 5s^2 \ ^1S_0$ transition in ^{87}Sr atoms. Theoretical formulas and numerical results for decay rate have been obtained which can be used to estimate spectroscopic characteristics of this narrow-line in connection with the optical frequency standards.

The present study may be important for further experimental investigation on the other alkaline-earth Mg and Ca atoms, where the experimental accuracy can be improved considerably [2].

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5. REFERENCES

- [1] T.P. Dinneen, K.R. Vogel, E. Arimondo, J.L. Hall and A. Gallagher, Phys. Rev. Vol. 59A, pp. 1216-1222, 1999.
- [2] T. Binnewies, G. Wilpers, U. Sterr, F. Riehle, J. Helmcke, T.E. Mehlsträubler, E.M. Rasel and W. Ertmer, Phys. Rev. Lett. Vol. 87, pp. 123002-4, 2001.
- [3] E.H.Katori, T.Ido, Y.Isoya and M.K-Gonokami, in Atomic Physics 17, ed. E.Arimondo, P.DeNatale and M.Inguscio (AIP, New York, 2001), pp.382-396.
- [4] E.H.Katori, 2002, private communication.
- [5] I.P. Grant, C.F. Fischer and F.A. Parpia, GRASP-1992, private communication.
- [6] A. Derevianko, Phys. Rev. Lett. Vol. 87, pp. 023002-4, 2001.
- [7] L. Rayleigh, Proc. R. Soc. London. Vol.117A, pp.294-298, 1927.
- [8] M. Fukuda, Vol.4, pp.171-180, 1926.
- [9] R.H. Garstang, Vol. 81, pp.488-512, 1969.
- [10] P.J. Mohr, in "Beam-Foil Spectroscopy", eds. I.A. Sellin and D.J. Pegg (Plenum, New York, 1976), pp.97-115.
- [11] H.J. Kluge and H. Sauter, Z.Phys., Vol. 270, pp.295-309, 1974.
- [12] N.L. Manakov, V.D. Ovsiannikov and L.P. Rapoport, Phys. Rep., Vol.141, pp.319-321, 1986.
- [13] V.G. Pal'chikov, Hyperfine Interaction, Vol.127, pp.287-292, 2000