Physics Letters A 379 (2015) 1347–1353

Contents lists available at ScienceDirect

Physics Letters A

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A simplified method for calculating the ac Stark shift of hyperfine levels of alkali-metal atoms

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ARTICLE INFO

Article history:
Received 12 September 2014
Received in revised form 18 March 2015
Accepted 20 March 2015
Available online 23 March 2015
Communicated by V.A. Markel

Keywords:
ac Stark shift
Hyperfine structure
Differential light shift
Microwave clocks
Green's function

ABSTRACT

The ac Stark shift of hyperfine levels of neutral atoms can be calculated using the third order perturbation theory (TOPT), where the third order corrections are quadratic in the atom–photon interaction and linear in the hyperfine interaction. In this paper, we use Green's function to derive the $E^{[2+\epsilon]}$ method which can give close values to those of TOPT for the differential light shift between two hyperfine levels. It comes with a simple form and easy incorporation of theoretical and experimental atomic structure data. Furthermore, we analyze the order of approximation and give the condition under which $E^{[2+\epsilon]}$ method is valid.

1. Introduction

The recent developments in precision measurement [1,2] and optical communication [3] require a possible way to calculate the ac Stark shift with considerable precision. In many cases, the second order perturbation theory (SOPT) [4], which is capable of utilizing the existing theoretical and experimental atomic structure data, is used to compute the light shifts. For instance, in today's researches on atomic clocks, it has been realized that the accuracy and stability can be substantially improved by trapping cold atoms in a standing wave of light (optical lattice) [5,6]. Because of the minimization of Doppler and recoil effects, light shift caused by trapping laser is essential. Therefore the wavelength of the trapping laser should be tuned to a region where the light shifts of the two clock transition states cancel each other out. This wavelength is called "magic wavelength" [7]. In optical clocks and terahertz clocks, the clock transition is between the fine structure of atomic ground state and excited states, and we can utilize the SOPT to compute the light shift of the clock transition. The shift arises in the second order of perturbation theory which is quadratic in the electric field strength. The calculations suggest the existence of magic wavelength both for optical-clock transitions [8,9] and terahertz-clock transitions [10].

Recently, the alkali-metal atom like rubidium (Rb) and cesium (Cs) are considered as potential choices for microwave lattice clocks, using the two field insensitive hyperfine levels of the ground state as clock transition levels [11]. However, because SOPT doesn't take into account the hyperfine interaction, the results are identical for the hyperfine doublet of the ground state at arbitrary values of trapping laser wavelength. To solve this problem, the third order perturbation theory (TOPT) [16–18] was proposed by extending the formalism to the higher order of perturbation theory, and the third order corrections are quadratic in the field amplitude and linear in the hyperfine interaction. The theory requires using *ab initio* approach to construct the atomic structure database. Here we introduce the $E^{[2+\epsilon]}$ method which takes the hyperfine interactions into consideration in SOPT. We will show that for a wide range of trapping laser wavelength, $E^{[2+\epsilon]}$ method gives close results to those of TOPT and experiments. In addition, $E^{[2+\epsilon]}$ method comes with a simple form, easy incorporation of theoretical and experimental atomic structure data, and therefore is more applicable for other elements.

The remainder of this manuscript is organized as follows. We use Green's function and diagrammatic representation to derive the $E^{[2+\epsilon]}$ method in Section 2. In addition, we provide another derivation process in the form of formulas in Appendix A. In Section 3, the differential light shifts between two field insensitive hyperfine levels of the ground state of Cs and Rb are calculated using both methods, due to their potential application in microwave lattice clocks. In the calculation, besides utilizing the existing ex-

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http://dx.doi.org/10.1016/j.physleta.2015.03.024
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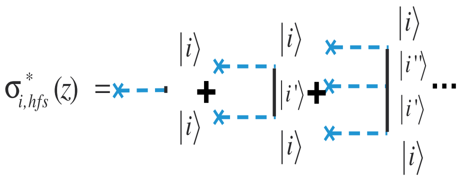

Fig. 1. (Color online.) Diagrammatic representation of $\sigma^*_{\mathrm{i,hfs}}(z)$. $|i'\rangle$ and $|i''\rangle$ denote different eigenstates of H_{fs} which have the same parity with $|i\rangle$ but with different J or principle quantum numbers. Every solid line (black) marked by $|i\rangle$ represents a factor $g^0_i(z) = 1/(z - \langle i|H_{\mathrm{fs}}|i\rangle)$. Every dashed line (blue) marked by $|i\rangle$ and $|i'\rangle$ denotes a factor $\langle i|H_{\mathrm{hfs}}|i'\rangle$. A summation is performed over the index $i', i'' \ldots$ in the end, where $i', i'' \neq i$.

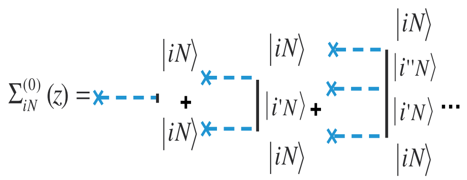

Fig. 2. (Color online.) Diagrammatic representation of $\Sigma^{(0)}_{\mathrm{iN}}(z)$. $|i'\rangle$ and $|i''\rangle$ denote different eigenstates of H_{fs} which have the same parity with $|i\rangle$ but with different J or principle quantum numbers. Every solid line (black) marked by $|iN\rangle$ represents a factor $G^0_{\mathrm{iN}}(z) = 1/(z - \langle iN|H_0|iN\rangle)$, and every dashed line (blue) marked by $|iN\rangle$ and $|i'N\rangle$ denote a factor $\langle iN|H_{\mathrm{hfs}}|i'N\rangle = \langle i|H_{\mathrm{hfs}}|i'\rangle$. A summation is performed over the index $i', i'' \ldots$ in the end, where $i', i'' \neq i$.

perimental atomic structure data, we use GraspVU code [12] to construct our own database of atomic structure, which is summarized in Appendix A. The discussions and conclusions are given in Section 4.

2. $E^{[2+\epsilon]}$ method

2.1. Hyperfine structure

We start with no light fields. The Hamiltonian h of the system can be written as the sum of the unperturbed part h_0 and the perturbation Δh.

$$
\begin{aligned}
h &= h_0 + \Delta h, \\
h_0 &= H_{\mathrm{fs}}, \\
\Delta h &= H_{\mathrm{hfs}}.
\end{aligned}
\tag{1}
$$

Here h_0 is the fine structure Hamiltonian H_{fs}, and the perturbation Δh is the hyperfine interaction Hamiltonian H_{hfs}. In the coupled representation, the eigenstate of H_{fs} can be written as

$$
|nIJFM_F\rangle = \sum_{M_J, M_I} \langle JM_J IM_I|FM_F\rangle \times |nJM_J\rangle|IM_I\rangle, \tag{2}
$$

where n is the principle quantum number, I is the nuclear spin, J is the electronic total angular momentum and $F = I + J$ is the total angular momentum; M_I, M_J and M_F are the projections of I, J and F on the quantization axis, respectively. $\langle JM_J IM_I|FM_F\rangle$ is the Clebsh–Gordan coefficient. However, Eq. (2) is not an eigenstate of h, because the hyperfine interactions have non-zero off-diagonal matrix elements. In the following, we use a shorthand notation $|i\rangle \equiv |n_i I J_i F_i M_{Fi}\rangle$ for convenience.

The resolvent of h with complex variable z is

$$
g_{\mathrm{n_i,i}}(z) = \langle i|\frac{1}{z-h}|i\rangle = \frac{1}{z - E_{\mathrm{i,fs}} - \sigma^*_{\mathrm{i,hfs}}(z)}, \tag{3}
$$

where $\sigma^*_{\mathrm{i,hfs}}(z)$ is the expectation value of the level-shift operator in the state $|i\rangle$, which can be diagrammatically represented by the Brillouin–Wigner perturbation series in Fig. 1. Because the hyperfine state energy $E_i = E_{\mathrm{i,fs}} + E_{\mathrm{i,hfs}}$ is one pole of the Green's function, where $E_{\mathrm{i,fs}}$ and $E_{\mathrm{i,hfs}}$ are the fine structure energy and the hyperfine corrections, respectively, we have:

$$
E_{\mathrm{i,hfs}} = \sigma^*_{\mathrm{i,hfs}}(E_{\mathrm{i,fs}} + E_{\mathrm{i,hfs}}) = \sigma^*_{\mathrm{i,hfs}}(E_i). \tag{4}
$$

2.2. The ac Stark shift

Now we consider a neutral atom in a far-off-resonance laser field with frequency $\nu = \omega/2\pi$. The laser field is assumed to be in a Fock state $|R\rangle = |N\rangle$ ($N \gg 1$), where N equals the mean photon number. The Hamiltonian H of the system can be written as the sum of the unperturbed part H_0 and the perturbation ΔH:

$$
\begin{aligned}
H &= H_0 + \Delta H, \\
H_0 &= H_R + H_{\mathrm{fs}}, \\
\Delta H &= H_{\mathrm{hfs}} + H_e.
\end{aligned}
\tag{5}
$$

Here H_0 consists of the radiation field Hamiltonian H_R and the fine structure Hamiltonian H_{fs}. The state $|iN\rangle \equiv |i\rangle \otimes |N\rangle$ is an eigenstate of H_0 with eigenvalue $E_{\mathrm{i,fs}} + N\hbar\omega$.

The perturbation ΔH of Eq. (5) takes into account the hyperfine interaction H_{hfs} and atom–photon interaction H_e. For H_e, we use the dipole approximation $H_e = -d\cdot\vec{\varepsilon}$, where d is the electric dipole moment and $\vec{\varepsilon}$ is the electric field vector. Here for the sake of simplicity, we have ignored the atom's external degree of freedom.

The resolvent of H with complex variable z has a similar form to Eq. (3):

$$
G_{\mathrm{iN}}(z) = \langle iN|\frac{1}{z-H}|iN\rangle = \frac{1}{z - E_{\mathrm{i,fs}} - N\hbar\omega - \Sigma^*_{\mathrm{iN}}(z)}, \tag{6}
$$

with the expectation value of the level-shift operator in the state $|iN\rangle$

$$
\Sigma^*_{\mathrm{iN}}(z) \approx \Sigma^{(0)}_{\mathrm{iN}}(z) + \Sigma^{(2)}_{\mathrm{iN}}(z), \tag{7}
$$

where $\Sigma^{(0)}_{\mathrm{iN}}(z)$ and $\Sigma^{(2)}_{\mathrm{iN}}(z)$ are the parts containing the 0th and 2nd order of H_e, respectively. Here we have neglected higher orders of atom–photon interactions, due to the reasons presented in the discussion.

The terms in $\Sigma^{(0)}_{\mathrm{iN}}(z)$ and $\Sigma^{(2)}_{\mathrm{iN}}(z)$ can also be represented diagrammatically. In Fig. 2, $\Sigma^{(0)}_{\mathrm{iN}}(z)$ has a similar structure to that of $\sigma^*_{\mathrm{i,hfs}}(z)$ except the solid lines represent $G^0_{\mathrm{iN}}(z) = 1/(z - \langle iN|H_0|iN\rangle)$, not $g^0_i(z) = 1/(z - \langle i|H_{\mathrm{fs}}|i\rangle)$. The diagrams of $\Sigma^{(2)}_{\mathrm{iN}}(z)$ are more complicated. It can be decomposed into three kinds of factors: C, D and H, which are presented in Fig. 3:

$$
\Sigma^{(2)}_{\mathrm{iN}}(z) = \sum_{\substack{i',i''\\ j',j''}} C^{\mathrm{i''N}}_{\mathrm{iN}} \cdot H^{\mathrm{i''N}}_{\mathrm{j''N\pm1}} \cdot D^{\mathrm{j''N\pm1}}_{\mathrm{j'N\pm1}} \cdot H^{\mathrm{j'N\pm1}}_{\mathrm{i'N}} \cdot C^{\mathrm{i'N}}_{\mathrm{iN}} \tag{8}
$$

As shown in the diagram, the hyperfine interactions are included in the C and D factors, meanwhile the H factor contains the atom–photon interactions. The factors C and D are very similar, except in $C^{\mathrm{i'N}}_{\mathrm{iN}}$, $|i\rangle$ cannot be an intermediate state, meanwhile in $D^{\mathrm{i'N}}_{\mathrm{iN}}$ there is no such restriction. We can calculate the C, D and H factors formally:

$$
\begin{aligned}
C^{\mathrm{i'N}}_{\mathrm{iN}} &= \delta_{\mathrm{i,i'}} + (1 - \delta_{ii'})\frac{1 - G^0_{\mathrm{iN}}\Sigma^{(0)}_{\mathrm{iN}}}{G^0_{\mathrm{iN}}} D^{\mathrm{i'N}}_{\mathrm{iN}} \\
D^{\mathrm{j'N}}_{\mathrm{jN}} &= [\delta_{\mathrm{j,j'}} + (1 - \delta_{jj'})C^{\mathrm{j'N}}_{\mathrm{jN}}]\frac{G^0_{\mathrm{jN}}}{1 - G^0_{\mathrm{jN}}\Sigma^{(0)}_{\mathrm{jN}}} \\
H^{jN\pm1}_{\mathrm{iN}} &= \langle jN \pm 1|H_e|iN\rangle
\end{aligned}
\tag{9}
$$