Theoretical calculation of saturated absorption spectroscopy of atomic ytterbium beam

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Abstract. Saturated absorption spectroscopy is a technique of measuring the transmission of a probe beam induced by a counter-propagating pump beam, which can achieve a nearly Doppler-free spectral resolution. In this study, the saturated absorption spectra of individual isotopes of ytterbium atoms are calculated using rate equations for various polarizations of the probe and pump beams under an assumption that the distribution of velocities for atoms within the atomic beam is a Maxwell-Boltzmann distribution. The fourth-order Runge-Kutta method is used for calculation of the rate equations, then the absorption coefficient in the vicinity of the atomic transitions is calculated, and the transmission of the probe beam is obtained by Beer-Lambert law. We compare the calculations with an experimental result from the literature and obtain a good agreement.

1. Introduction

Saturated absorption spectroscopy is a common technique in atomic physics that allows observing near-natural linewidth of atomic transitions. The principle of saturated absorption spectroscopy is sending counter-propagating pump and (low intensity) probe beams through atomic vapor at the same frequency. Wide and deep dips of intensity, which belong to the Doppler-broadened absorption, are observed when the frequency of the pump beam is swept across atomic resonances. Since the strong pump beam can excite the majority of atoms, the probe beam is no longer absorbed by the atoms. Once the frequency of the probe beam is swept, a small peak in transmission is observed at each hyperfine transition. Previously, solutions for the saturated absorption spectra can be solved analytically and numerically for an element that has only a single stable isotope or each isotope having no overlapping transitions using the rate equation model [1]. However, ytterbium, a candidate for providing a frequency reference, has overlapping peaks in the spectrum for the $^{173}$Yb($F=3/2$), $^{172}$Yb and $^{173}$Yb($F=7/2$) [2]. In this case, it is interesting to prove that this method can still provide an acceptable result.

In this research, saturated absorption spectra of individual isotopes of ytterbium are calculated using rate equations for various polarizations of the probe and pump beams which are introduced in references [1, 3]. The fourth-order Runge-Kutta method is used for calculations
of the rate equations, and the transmission of the probe beam is obtained and compared with the experimental result from T. Loftus et al. [4].

2. Rate equation

Rate equations are equations that describe the exchange of population between states of an atom in the presence of laser beams. In this case, the intensity of the probe beam is relatively weak compared to the intensity of the pump beam, so the effect of the probe beam in the coupling between states of the atom is ignored. The pump beam couples hyperfine levels in the ground and excited states. The quantum numbers \( F = F_g \) and \( F = F_e \) indicate total atomic angular momentum of the ground state and excited state, respectively, and sub-levels are indicated by \( m = m_g \) and \( m = m_e \) which is the projection of the angular momentum of the ground state and excited state along the quantization axis. Three types of polarization of the pump beam are indicated by \( q_{pump} \), where \( q_{pump} = \pm 1 \) for left- and right- \((\sigma^{\mp})\) circularly polarized beam and \( q_{pump} = 0 \) for linearly polarized \((\pi)\) beam, respectively. In general, we consider a multilevel atom with \( n \) ground states with populations \( P_{F_g}\), \( P_{F_g}^{m_g} \), \( P_{F_g}^{m_g} \), ..., \( P_{F_g}^{m_g} \) that share a common excited state with population \( P_{F_e}^{m_e} \). The rate equations for each individual ground state \( F_g \) with sub-levels \( m_g = -F_g, ..., F_g \) are given by [1, 3]

\[
\begin{align*}
\frac{dP_{F_g}^{m_g}}{dt} &= - \sum_{F_e=F_g-1}^{F_e=F_g+1} R_{F_g, m_g}^{F_e, m_g+q_{pump}} \frac{\Gamma s_0}{2} \left\{ P_{F_g}^{m_g} - P_{F_g}^{m_g+q_{pump}} \right\} \\
&+ \sum_{F_e=F_g-1}^{F_e=F_g+1} \sum_{m_e=m_g+1}^{m_e+1} \Gamma R_{F_g, m_g}^{F_e, m_e} P_{F_e}^{m_e}.
\end{align*}
\]

Here, \( s_0 = I_L / I_{sat} \), where \( I_L \) is the intensity of incident laser beam; \( I_0 \) is the saturation intensity. \( \delta_{pump} = \delta + kv \) is the pump beam’s frequency experienced by the atom, where \( \delta \) is the detuning of the pump beam, \( v \) is the velocity of the atom, and \( k \) is the wavenumber. \( \Gamma \) is the natural linewidth, and \( \Delta_{F_e+1}^{F_e} \) is the zero-field hyperfine frequency separations. The rate equations for the excited state \( F_e \) with sub-levels \( m_e = -F_e, ..., F_e \) are given by

\[
\begin{align*}
\frac{dP_{F_e}^{m_e}}{dt} &= R_{F_g, m_g}^{F_e, m_e-q_{pump}} \frac{\Gamma s_0}{2} \left\{ P_{F_g}^{m_g-q_{pump}} - P_{F_g}^{m_g} \right\} - \sum_{j=1}^{n} \sum_{m_g=m_e-1}^{m_e+1} \Gamma R_{F_g, m_g}^{F_e, m_e} P_{F_e}^{m_e}.
\end{align*}
\]

The number \( R_{F_g, m_g}^{F_e, m_e} \) is the normalized line strength for the atom that depends on the total nuclear angular momentum \( I \), the total spin angular momentum \( S \), the total angular momentum \( J \), and the total orbital angular momentum \( L \) given by

\[
R_{F_g, m_g}^{F_e, m_e} = (2L_e + 1)(2J_g + 1)(2J_e + 1)(2F_g + 1)(2F_e + 1)
\times \left[ \begin{array}{c} 1 \\ m_g \\ q_{pump/probe} \\ -m_e \end{array} \right] \left[ \begin{array}{c} J_g \\ J_e \\ 1 \\ F_g \\ F_e \\ I \end{array} \right] \left[ \begin{array}{c} L_g \\ L_e \\ 1 \\ J_e \\ J_g \\ S \end{array} \right]^2.
\]

where the subscripts \( g \) and \( e \) refer to ground state and excited state, respectively. The term in round bracket is the Wigner 3-j symbol and the terms in curly brackets are the Wigner 6-j symbols. Finally, \( q_{pump/probe} \) indicates the type of polarization of pump beam or probe beam.

In this work, rate equations of \(^{1}S_0 \rightarrow ^{1}P_1\) transition for six isotopes of ytterbium include \(^{170}\text{Yb}, \quad Yb, \quad ^{172}\text{Yb}, \quad ^{173}\text{Yb}, \quad ^{174}\text{Yb} \) and \(^{176}\text{Yb} \) are calculated using the fourth-order Runge-Kutta
method individually. However, the spectrum of $^{168}$Yb cannot be observed in the experiment because of its very low natural abundance. In the absence of the pump beam, we assume that initially atomic populations are equally distributed in sub-levels of the ground state. All associated parameters in the experiment are obtained from reference [4]. Figure 1 shows all possible transitions of ytterbium isotopes which can be excited by the pump beam. Figure 2 shows the sample calculation results using the fourth-order Runge-Kutta method for $\pi$ pump beam which couples $^1S_0$ ($F_g = 0, m_g = 0$) sub-level and $^1P_1$ ($F_e = 1, m_e = 0$) sub-level of $^{174}$Yb. The laser detuning is given by $\Delta_{174} = \nu_L - \nu_{174}$, where $\nu_L$ is the laser frequency and $\nu_{174}$ is the $^{174}$Yb $^1S_0 - ^1P_1$ resonance frequency.

Figure 1. Energy levels of ytterbium: (a) fermionic isotope ($^{173}$Yb) (b) fermionic isotope ($^{171}$Yb) and (c) bosonic isotopes ($^{168}$Yb, $^{170}$Yb, $^{172}$Yb, $^{174}$Yb and $^{176}$Yb), where linearly polarized ($\pi$) pump beam is used to couple two sub-levels with $\Delta m = 0$.

Figure 2. Comparision between calculation results for $^{174}$Yb using the fourth-order Runge-Kutta method and the analytical solutions of the rate equations for $\pi$ pump beam which couples (a) $^1S_0$ ($F_g = 0, m_g = 0$) and (b) $^1P_1$ ($F_e = 1, m_e = 0$) sub-level.
3. Saturated absorption spectroscopy

From Beer-Lambert law, the transmission of a laser beam through an atomic vapor is given by

\[ T(\delta) = e^{-\alpha(\delta)L_p}, \]  

(4)

where \( L_p \) is path length of the laser beam through the atomic vapor and \( \delta \) is detuning of laser frequency from the atomic transition resonance. The absorption coefficient is given by [5]

\[ \alpha(\delta) = \int_{-\infty}^{\infty} n_{atom} f(v) \sigma(\delta, v) \, dv, \]  

(5)

where \( n_{atom} \) is the atomic density, \( f(v) \) is the velocity distribution of the atoms, \( \sigma(\delta, v) \) is the absorption cross-section. The transmission of probe beam in the presence of a pump beam which is tuned to the resonance frequency is calculated under two assumptions: the distribution of velocities for atoms within the atomic beam is a Maxwell-Boltzmann distribution, and the effect of probe beam on exciting the atom can be neglected because of its weak intensity. The transmission of probe beam with the Doppler background signal subtracted is given by [1]

\[
T(\delta) = -\int_{-\infty}^{\infty} dv \frac{3\lambda^2}{2\pi} n_{atom} L_p e^{-\left(v/v_{mp}\right)^2} \frac{\delta_{probe}}{1 + 4 \left(\delta_{probe} + \Delta F_{g,e}^{F_g,F_e^{m_g,q_{probe}}} + \Delta F_{g,e}^{m_g}\right)^2 / \Gamma^2},
\]

(6)

where \( \lambda \) is the wavelength of transition, \( \delta_{probe} = \delta - kv \) is the probe beam’s frequency experienced by the atom, \( v_{mp} = \sqrt{2k_B T/m} \) is the most probable velocity of the atoms with mass \( m \) at temperature \( T \), and \( k_B \) is Boltzmann constant. The polarizations of the probe beam are denoted by \( q_{probe} = \pm 1 \) and 0 for the \( \sigma^\pm \) and \( \pi \) transitions, respectively. \( P_g \) is the number which represents the population of each ground-state sub-level without the pump beam.

![Figure 3](image-url)  

Figure 3. Comparision between the calculation result from equation (6) of \(^1S_0 - ^1P_1\) transition for six isotopes of ytterbium and the experimental data extracted from reference [4], where CO1 and CO2 are crossover resonances of \(^{173}\text{Yb}\) and \(^{171}\text{Yb}\), respectively.
According to the experiment of T. Loftus et al. in 2001, the polarizations of pump beam and probe beam are not defined. Thus, the pump beam and probe beam polarizations are assumed to be linear as a typical polarization of light in an experiment; the pump beam intensity is stronger than the saturation intensity \( s_0 \approx 2 \). The total spectrum is a superposition of spectra from individual isotopes. The calculation results in equation (6) for \( \pi \) transition of six isotopes of ytterbium are compared with the reference [4], and crossover resonances are also obtained for \(^{171}\text{Yb}\) and \(^{173}\text{Yb}\), as showed in figure 3. According to figure 3, the calculation and the experimental data do not match perfectly. This is due to the fact that we can not obtained all associated factors: intensity of pump beam, external magnetic field, laser intensity fluctuation while laser frequency scanning, and polarizations of pump beam and probe beam that affect the spectral profile and the amplitude of each peak.

4. Conclusion

In this research, the rate equations of each isotope of ytterbium are solved individually by the fourth-order Runge-Kutta method. The calculation results agree with analytical solutions for \(^{174}\text{Yb}\). The calculated population for each state of the isotopes are used to solve equation (6) numerically, and results show a good agreement with experimental data from T. Loftus et al. However, the calculation shows some deviation from the experimental result due to inaccessibility of experimental data obtained from reference [4]. Effects of polarization of probe beam and pump beam on changing the shape of spectrum of atomic gas is very strong as seen in rubidium [6]. Additionally, effect of intensity of pump beam and external magnetic field can be seen in cesium [7]. Thus, the laser beams should be well collimated to maintain the constant intensity, and magnetic compensation coils or magnetic shields might be required in order to cancel earth’s magnetic field. The accuracy of this method need to be proved again after conducting of an experiment under controlled and known factors. In summary, this method is applicable to obtain numerical calculations of the saturated absorption spectra for atoms with various isotopes and having overlapping transitions.

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