Study of factors affecting the light shift of the CPT resonance

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Abstract. Motivated by recent developments in atomic frequency standards employing the effect of coherent population trapping (CPT), we propose a theoretical framework for describing the CPT resonances. Our extended model includes several realistic experimental factors not accounted for in the standard approaches, namely, the FM-based technique for generating the error signal, skewed laser spectrum, etc. We provide a simple yet non-trivial analytical solution revealing the magnitude and structure of the light shift. The performance of the model is checked against numerical simulations, the agreement is good to perfect.

1. Introduction

The effect of coherent population trapping (CPT) allows to realize narrow resonances [1, 2, 3] and therefore is widely used in frequency standards and quantum metrology. In a single-source CPT-based atomic clock, a local microwave oscillator to be stabilized is involved in modulation of the optical carrier generating two sideband frequencies resonant with the shoulders of the atomic Λ-scheme, see Fig. 1(a). As long as the difference between these two frequencies is exactly $\omega_g$, the excited states are sparsely populated and the probing light experiences virtually no absorption. Fluctuations of the oscillator’s frequency destroy the resonance and lead to an increased light loss through the atomic cell. The feedback loop adjusting the oscillator to the atomic frequency $\omega_g$ is governed by the in-phase signal obtained by an additional slow modulation of the probing field. A side effect of such setup with a single laser source is a comb of different-order sidebands, each causing its own dynamic Stark shift of the atomic levels. Unless these partial shifts offset one another, a drift and/or fluctuations in the clock output due to random light power fluctuations occur. The current presentation focuses on the factors affecting the CPT resonance and especially the magnitude and structure of the light shift in a realistic experimental setting. The nomenclature of these factors is wider than in standard studies of this kind [4, 5]: we take into account slow modulation providing the error signal, allow for a skewed laser spectrum, consider a four-level structure of $D_1$-line in $^{87}$Rb atoms, an arbitrary one-photon detuning and optically thick atomic medium.
2. Model
Consider the $D_1$-line of $^{87}$Rb atoms interacting with $\sigma_+$-polarized light, see Fig. 1(a). The light field is obtained by modulating the injection current of a laser with a microwave frequency of the local oscillator $\Omega \approx \omega_g/2$:

$$\frac{E_0}{2} e^{-i\omega t} \sum_n A_n e^{-i\Phi(t)} + c.c. \quad (1)$$

In (1), $\Phi(t) = \Omega t + b \sin \omega_m t$, amplitudes $A_n$ can be arbitrary, see Fig. 1(b), the carrier $\omega = \omega_0 + \Delta_L$ can be slightly detuned from the optical frequency $\omega_0$ by quantity $\Delta_L$.

![Diagram](image)

**Figure 1.** (a) Four-level structure of $D_1$-line of $^{87}$Rb atoms. The parameters used in the presentation: $\Gamma/2\pi = 260$ MHz, $\Gamma_{ab}/2\pi = 150$ Hz, $\omega_m/2\pi = 90$ Hz, $b = 0.5$, total light power $P = 55 \mu$W, $\gamma_1/\Gamma = 0.018$, $\Delta_L = -\omega_e/4$, $\omega_g/2\pi = 3.417$ GHz, $\omega_e/2\pi = 816$ MHz, $d_0 = d_1/\sqrt{3}$, $\gamma_2 = \gamma_1/3$. To make the effects due to spectrum asymmetry observable, a sufficiently large value of $\Delta_L = -\omega_e/4$ is picked. (b) Experimental spectra involved in the demonstrations (labels correspond to the power of microwave modulation, in decibel per $\mu$W).

The instantaneous frequency, $\Phi'(t) = \Omega + b \omega_m \cos \omega_m t$, changes harmonically about a constant value $\Omega \equiv \omega_g/2 + \delta$ at a much slower rate $\omega_m$ with a small amplitude $b \omega_m$. A small scanning detuning $\delta$ is used to explore the resonant behavior of the system or can model a drift/fluctuation of the local oscillator from the benchmark frequency $\omega_g/2$. The first-order sideband frequencies $\omega \mp \Omega$ are close to resonance with the transitions $|a\rangle$ $\leftrightarrow |b\rangle$, and $|c_j\rangle$, $j = 1, 2$, and thus maintain the CPT effect. The modulation at $\omega_m$ provides a signed error signal used in the feedback loop of the atomic clock. Note that the microwave frequency $\Omega/2\pi \approx 3.4$ GHz exceeds $\omega_m/2\pi \sim 100$ Hz by seven orders of magnitude giving a chance for an analytical treatment of such two-scale problem.

3. Equations and approach
To describe the model theoretically, we employ the equations for the atomic density matrix $\dot{\rho}(t) = \sum_{\alpha,\beta} (|a\rangle\langle b| + |b\rangle\langle c| + |c_1\rangle\langle c_2|) \rho^{a\beta}(t) |\alpha\rangle \langle \beta|$

$$i \left( \frac{d}{dt} + \hat{\Gamma} \right) \dot{\rho} = [\hat{H}, \rho], \quad (2)$$
The Hamiltonian is written under the resonant approximation with respect to the carrier frequency $\omega$ with the interaction terms $V_j(t) = \sum_n V_{j,n} e^{-i\Phi(t)}$, $V_{j,n} = \frac{d_j E_0}{2} A_n$ where $d_j = d_j^+ = \langle a | d | c_j\rangle = \langle b | d | c_j\rangle$, $j = 1, 2$, are the dipole matrix elements assumed real and equal for both shoulders of the $\Lambda$-scheme.

The relaxation operator in (2) reads: $\hat{\Gamma} \equiv \hat{\Gamma}_c + \hat{\Gamma}_{ab}$, where

$$\hat{\Gamma}_c \hat{\rho} = \sum_{j=1}^2 \gamma_j \rho^{c_j c_j} \left( |c_j\rangle \langle c_j| - \frac{1}{2} \{ |a\rangle \langle a| + |b\rangle \langle b| \} \right) + \Gamma \left\{ \rho^{a(b以外のレベル)|c_j\rangle \langle c_j|} |b\rangle + \text{h.c.} \right\}$$

and $\hat{\Gamma}_{ab \hat{\rho}} = \Gamma_{ab} \{ \rho^{ab} |a\rangle \langle b| + \text{h.c.} \}$. It describes the incoherent phenomena of three kinds: (i) pumping the ground levels due to radiative decay from the upper states at the individual rates $\gamma_j$ (ii) decay of the coherences $\rho^{c_j a}$, $\rho^{c_j b}$ at a rate of $\Gamma \gg \gamma_j$ due to collisions with the buffer gas, and (iii) slow relaxation of coherence between the ground sublevels at a rate $\Gamma_{ab}/2 \pi \sim 150$ Hz (term $\Gamma_{ab}$).

Following the structure of the interaction term $V_j(t)$, the density matrix is sought in the form of series:

$$\rho^{\alpha\beta}(t) = \sum_{n=-\infty}^{\infty} \rho_n^{\alpha\beta}(t) \exp(-i n \Omega t), \quad \alpha, \beta = \{ a, b, c_1, c_2 \},$$

where the amplitudes $\rho_n^{\alpha\beta}(t)$ are supposed to change at a characteristic rate $\omega_m$, i.e., very slowly compared to the microwave scale $\Omega$. Projecting equations (2) onto the basis $\exp(-i n \Omega t)$, we get the equations for amplitudes in (4). In doing so, we treat the slow quantities $\rho_n^{\alpha\beta}(t)$, $V_{j,n}(t)$ as constants neglecting errors $\sim \omega_m/\Omega \sim 10^{-7}$. Furthermore, the light is assumed weak

$$d_j E_0/2\hbar \ll \gamma_j \ll \Gamma \ll \Omega$$

which allows eliminate the excited levels adiabatically. As a result, we arrive at a set of two equations for the ground state populations $\rho_0^{aa}$, $\rho_0^{ab}$ (obeying $\rho_0^{aa} + \rho_0^{bb} \approx 1$), and the coherence between them $\rho_2^{ab}$:

$$\frac{d\rho_0^{aa}}{dt} + 2\lambda \rho_0^{aa} = 2A \text{Im} \rho_2^{ab} + f_{aa},$$

$$i\frac{d\rho_2^{ab}}{dt} + (2b \omega_m \cos \omega_m t + 2\Delta + i\Gamma_{ab} + 2i\lambda) \rho_2^{ab} = 2A \rho_0^{aa} + f_{ab},$$

and an equation for the total population of the upper levels:

$$\rho_0^{c_1 c_1}(t) + \rho_0^{c_2 c_2}(t) = f_{cc} + 2C \text{Re} \rho_2^{ab}(t) + D \rho_0^{aa}(t),$$

with the coefficients collected in Appendix. Even though the population of the upper levels (7) is small under the CPT resonance, it is a quantity of primary interest as it determines the light absorption in the atomic cell, $M_0 = \langle \rho_0^{c_1 c_1}(t) + \rho_0^{c_2 c_2}(t) \rangle$, as well as the response to the modulation at the frequency $\omega_m$, $M_f = \langle (\rho_0^{c_1 c_1}(t) + \rho_0^{c_2 c_2}(t)) \times \cos \omega_m t \rangle$, i.e., the in-phase signal. Brackets $\langle \ldots \rangle$ denote averaging over $\gtrsim \omega_m^{-1}$ sec.

Reduction (2) $\rightarrow$ (6) lowers the number of equations from ten to two, it is valid under conditions (5) and for arbitrary spectrum and detuning $\Delta_L$. Yet, system (6) needs to be solved
numerically because of a time dependent coefficient in (6b). Unlike the original equations (2) having two very different frequency scales $\omega_m$, $\Omega$ and thus requiring an extremely small time step throughout the entire integration, numerical solution of “slow” equations (6) is fast and easy but gives little analytic insight into qualitative dependence on the driving parameters. An additional assumption of small frequency deviation $b\omega_m \ll \lambda$ allows to find a steady-state solution to (6) analyzed below.

4. Results of simulation

Here we summarize the basic results obtained from the reduced equations (6). For a non-skewed spectrum $V_{j,-n}^2 = V_{j,n}^2$, the resonance line is a symmetric Lorentzian $\propto \Delta^2 / (\lambda' + \Delta^2)$, $\Delta = \delta - \delta_0^{(s)}$, with a width $\lambda' = \lambda + \Gamma_{ab}/2$ and centered at the point $\delta_0^{(s)}$:

$$
\delta_0^{(s)} = -\frac{1}{2} \sum_{j=1}^{2} \frac{\Delta_{L,j} \left( V_{j,1}^2 - V_{j,-1}^2 \right)}{\Delta_{L,j}^2 + \Gamma^2} - \frac{1}{2} \sum_{j=1}^{2} \sum_{n \neq 0} \frac{(n\Omega + \Delta_{L,j}) \left( V_{j,n+1}^2 - V_{j,n-1}^2 \right)}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2}.
$$

(8)

where $\Delta_{L,1} = \Delta_L$ and $\Delta_{L,2} = \Delta_L + \omega_e$. Displacement (8) defines a conventional light shift consisting of sub-shifts due to individual spectrum components. Note that the resonant shift $\delta_0^{(r)} = 0$ for the non-skewed spectrum.

Figure 2. The CPT resonance line and in-phase signal obtained from (6). Black crosses stand for numerical integration of the full system (2). The spectrum used in the simulation is labeled as $-8.2$ dbm in Fig. 1(b), $\Delta_L = -\omega_e/4$.

A skewed spectrum makes the resonance asymmetric, see, for example, Fig. 2. The light shift (minimizer of absorption) takes the form

$$
\delta_0 \approx \delta_0^{(s)} + \delta_0^{(a)},
$$

(9)

where the correction due to contour asymmetry reads

$$
\delta_0^{(a)} \approx \text{sign}(A_1^2 - A_{-1}^2) \frac{\lambda'}{2\lambda} \left[ 1 + \frac{2\lambda}{B\Gamma} |2\rho^{aa} - 1| \right] \sum_{j=1}^{2} \frac{\Delta_{L,j} V_{j,1} V_{j,-1}}{\Delta_{L,j}^2 + \Gamma^2},
$$

(10)
Table 1. Components of the light shift, in Hz. Structure of the cell: $\frac{\delta_0^{(r)}\delta_0^{(nr)}}{\delta_0^0}$ true. The value $\delta_0^{(r)}$ true comes from the numerical solution of (6). Value $\delta_0^{(nr)}$ is computed at $\Delta L, 1 = \Delta L, 2 = 0$ making unimportant (at $\Gamma^2 \ll \Omega^2$) whether the higher-order sidebands are symmetric.

| $\Delta L/\omega_o \rightarrow$ | RF power ↓ | -1    | -0.5 | -0.25 | 0    | 0.25 |
|-------------------------------|-----------|-------|------|-------|------|------|
| -10                           | -19\28   | -20\28 | -24\28 | 6\28 | 37\28|
| -9.2                          | 29\9\39  | 30\8\40 | 31\7\36 | 7\16 | 39\16|
| 25\5\30  | -25\5\16 | -21\16 | -25\16 | 7\16 | 39\16|
| -8.2                          | 35\5\23 | 35\5\23 | 35\5\23 | 7\16 | 39\16|
| -7.85                         | 43\5\23 | 43\5\23 | 43\5\23 | 7\16 | 39\16|
| -7.5                          | 44\5\23 | 44\5\23 | 44\5\23 | 7\16 | 39\16|
| -7                            | 45\5\23 | 45\5\23 | 45\5\23 | 7\16 | 39\16|

and exists as long as the first-order sidebands are different in absolute value. The term $\delta_0^{(a)}$ makes up a considerable part of the light shift, as shown in Table 1. The same Table demonstrates an accurate accuracy of formula (9) against the values obtained numerically from (6). Also, it reveals the contribution of each component of the light shift and suggests that the spectrum skewness is not important in the non-resonant shift, $\delta_0^{(r)} + \delta_0^{(nr)} \approx \delta_0^{(s)}$, despite the higher-order sidebands are asymmetric and the detunings $\Delta L, 1, \Delta L, 2$ are not small.

A list of other obtained results includes a statement about a point $\delta_0^{(in-ph)}$ where the in-phase signal turns to zero: it appears to be approximately equal to $\delta_0$ at $b \omega_m \ll \lambda$. There also exists a value of $\Delta L$ at which the above effects due to spectrum skewness almost disappear. A non-zero value of $\Gamma_{ab}$ makes the light shift (9) partially $E_d^2$-independent which might reduce to some extent the impact of random light fluctuations on the stability of the frequency standard. We also studied the effect of optically thick atomic medium (doing that rather phenomenologically than in a self-consistent way) and found a slight monotonic decrease of the light shift as the medium gets less transparent. Peculiarities of the resonance in the thick media were also discussed in [6, 7].

5. Conclusion
In summary, we proposed a model of the CPT resonance including a number of experimental factors that could influence on the value of the light shift and thus on the stability of the atomic clock. Among them we point out the spectrum skewness as a factor that can drastically change both the value and structure of the light shift not predictable by conventional formulae.

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Appendix A. Coefficients of (6),(7)

Coefficients of system (6),(7) are given by:

\[ \lambda = \frac{\Gamma}{2} \sum_{j=1}^{2} \sum_{n} \frac{V_{j,n+1}^2 + V_{j,n-1}^2}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2} \]

\[ A = - \sum_{j=1}^{2} \sum_{n} (n\Omega + \Delta_{L,j}) V_{j,n+1} V_{j,n-1} \frac{1}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2} \]

\[ D = - \sum_{j=1}^{2} \frac{2\Gamma}{\gamma_j} \sum_{n} \frac{V_{j,n+1}^2 - V_{j,n-1}^2}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2} \]

\[ C = \sum_{j=1}^{2} \frac{2\Gamma}{\gamma_j} \sum_{n} \frac{V_{j,n+1} V_{j,n-1}}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2} \equiv \frac{2\Gamma}{\gamma_1} B_1 + \frac{2\Gamma}{\gamma_2} B_2, \]

\[ f_{aa} = \sum_{j=1}^{2} \frac{\Gamma}{\gamma_j} \sum_{n} \frac{V_{j,n+1}^2}{(n\Omega + \Delta_{L,j})^2 + \Gamma^2} \equiv \Gamma (F_1 + F_2), \]

\[ f_{cc} = \frac{2\Gamma}{\gamma_1} F_1 + \frac{2\Gamma}{\gamma_2} F_2, \quad f_{ab} = - A - i\Gamma B, \quad B \equiv B_1 + B_2. \]