

# Alternative Variables for Computing Sideband Pulling in Atomic Frequency Standards

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**Abstract**—Sideband pulling has long been considered a possible source of frequency bias in atomic frequency standards. We treat a two-level system excited by coherent radiation with amplitude and phase modulation. We create alternative variables to facilitate the second-order solution of the associated time-dependent Schrödinger equation. We extend earlier work to include time-dependent excitation and initial phase dependence.

## I. INTRODUCTION

Frequency shifts due to the presence of sidebands on the exciting radiation have been of concern from the earliest days of atomic frequency standards [1]. Results valid for sidebands further removed from the carrier than the Rabi width were given long ago [2,3]. In 1978 Audoin et al. published a second-order result for the shift due to a single sideband valid for an arbitrary sideband separation [4]. Although this theory predicted a first-order shift, it was assumed to average to zero for the continuous signals from the atomic beam frequency standards of the time. Their result has been in use ever since to determine sideband intensity limits necessary to avoid a shift larger than other uncertainties.

With the advent of cesium fountains operating in pulsed modes, the possibility of modulation in synchronism with the cycling of the fountain signals was considered [5]. A deliberate application of synchronized phase modulation produced significant shifts in the primary standard NIST-F1 [6]. An accompanying theory agreed with the experimental results.

The purpose of the present paper is to extend the second-order results of Audoin et. al. to include contributions from synchronized pulsed operation and from two sidebands, equally spaced from the carrier, with arbitrary relative amplitudes and phases. Such sidebands may be re-expressed as the simultaneous application of amplitude and phase modulation at the same modulation frequency. We adopt this latter representation since amplitude and phase modulations interact with the dynamics of a two-level system in different manners. The primary focus of our analysis will be the dependence of any shifts on the initial phases of the modulations.

## II. BACKGROUND THEORY

We begin with a two-level system excited by an electromagnetic field proportional to

$$B = [b + b_a \cos(\Omega t + \varphi_a)] \cos[\omega t - (b_p / b) \sin(\Omega t + \varphi_p)],$$

where  $2b$  is the Rabi frequency for the excitation, and  $b_a$  and  $b_p$  are the corresponding Rabi frequencies for amplitude and phase modulation. These Rabi frequencies may be constant, or have time dependence. For half-sine-wave excitation we have  $b(t) = (\pi/2)b_0 \sin(\pi t / \tau)$ . We assume  $b_a$  and  $b_p$  have the same time dependence as  $b$ . For a single sideband  $b_a = b_p$  and  $\varphi_a - \varphi_p = 0$  or  $\pi$ . When the rotating wave approximation is made, and the probability amplitudes are redefined by appropriate time-dependent phases to eliminate the rapid  $\omega t$  time dependence [3,7], the resulting time-dependent Schrödinger equation for the system becomes

$$i\hbar \frac{d}{dt} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \hbar \begin{pmatrix} -\Delta & B_{\text{rot}}^* \\ B_{\text{rot}} & \Delta \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (1)$$

Here  $\Delta = \frac{1}{2}(\omega - \omega_0)$  is half the detuning from the atomic resonance  $\omega_0$  and  $*$  denotes the complex conjugate. The coupling by the field is now represented by the complex quantity

$$B_{\text{rot}} = (b + b_a \cos \theta_a) \exp[-i(b_p / b) \sin \theta_p].$$

We have introduced the abbreviations  $\theta_a = \Omega t + \varphi_a$  and  $\theta_p = \Omega t + \varphi_p$ . We impose on (1) the initial conditions at the beginning of excitation  $\alpha(t=0) = 1$  and  $\beta(t=0) = 0$ . Then  $\alpha$  is the probability amplitude that the system remains in its initial state and  $\beta$  is the probability amplitude that the system changes state. The Rabi transition probability is then  $P(t) = |\beta(t)|^2$ .

The corresponding Ramsey excitation probability is

$$P_{\text{Ram}} = |\beta_{\text{Ram}}|^2 = |\beta^{(2)}|^2 |\alpha^{(1)}|^2 + |\alpha^{(2)}|^2 |\beta^{(1)}|^2 + 2 \text{Re}(\gamma e^{2i\Delta T}),$$

where  $T$  is the period between the two excitations, and the coefficient  $\gamma$  is defined as

$$\gamma = \alpha^{(2)} \beta^{(2)} \alpha^{(1)} \beta^{(1)*}. \quad (2)$$

The superscripts refer to the first and second excitation regions, respectively. The two excitations are assumed identical, except that the initial phase of both modulations has advanced by  $\Phi \equiv \Omega(T + \tau)$  for the second excitation.

The presence of the perturbing modulations causes a frequency shift given by

$$2\Delta_{\text{res}} = \frac{\text{Im} \gamma}{T \text{Re} \gamma},$$

If we expand  $\gamma$ , defined by (2), in powers of the perturbation (subscripts) to second order, we find

$$2\Delta_{\text{res}} = \frac{\text{Im} \gamma_1}{T \text{Re} \gamma_0} + \frac{\text{Im} \gamma_2}{T \text{Re} \gamma_0} - \frac{\text{Im} \gamma_1 \text{Re} \gamma_1}{T (\text{Re} \gamma_0)^2}. \quad (3)$$

The imaginary part of  $\gamma_0$  was omitted because it is an odd function of  $\Delta$  and merely makes a small change in the value of  $T$  in the denominator (cf. Sec. 3.2 in [7]). Note that the first-order correction to the denominator makes a contribution in the last term. To find the perturbation expansion of  $\gamma$  we need the perturbation expansions of  $\alpha$  and  $\beta$ . These are difficult to derive from (1).

### III. ALTERNATIVE VARIABLES

To simplify the derivation of the perturbation expansion we define alternative variables as follows:

$$W(t) = e^{ia(t)} [\text{Re} \alpha(t) + i \text{Im} \beta(t)]$$

$$\text{and } Z(t) = e^{-ia(t)} [\text{Re} \beta(t) - i \text{Im} \alpha(t)],$$

where  $a(t)$  is defined as the integral of  $b(t)$ . The variables paired in the definitions are those coupled by the excitation. The exponentials in the definitions incorporate the unperturbed, on-tune evolution of the two level system. These new variables obey the same normalization criterion as  $\alpha$  and  $\beta$ :

$$|W(t)|^2 + |Z(t)|^2 = 1.$$

In terms of these variables the Rabi transition probability becomes

$$P = \frac{1}{2} - \frac{1}{2} \left[ \text{Re}(e^{-2ia} W^2) - \text{Re}(e^{2ia} Z^2) \right].$$

These alternative variables obey the following two differential equations:

$$dW / dt = -i\Delta e^{2ia(t)} Z + ib_a \cos \theta_a(t) W - b_p \sin \theta_p(t) e^{2ia(t)} Z$$

and

$$dZ / dt = -i\Delta e^{-2ia(t)} W - ib_a \cos \theta_a(t) Z + b_p \sin \theta_p(t) e^{-2ia(t)} W$$

where  $a(t)$  may be defined by a third simultaneous differential equation,

$$da / dt = b(t).$$

If these differential equations are multiplied by  $i$ , they form a Schrödinger-like pair with a two-by-two hermitian Hamiltonian. In the absence of detuning and the perturbation, the right-hand side vanishes. The variables  $W$  and  $Z$  then remain constant, equal to their initial conditions  $W(0) = 1$ ,  $Z(0) = 0$ . Solutions in powers of the perturbation reduce to straightforward integrals.

### IV. FIRST-ORDER SHIFTS

For small shifts of the Ramsey resonance we may ignore the detuning in the excitation regions. The first-order solution for  $W$  is then due only to amplitude modulation,

$$W_1(\tau) = -i \int_0^\tau b_a(t) \cos \theta_a(t) dt,$$

and for  $Z$  is due only to phase modulation:

$$Z_1(\tau) = \int_0^\tau b_p(t) \sin \theta_p(t) e^{-2ia(t)} dt.$$

Although the expressions for the real and imaginary parts of  $\gamma$  in terms of the alternative variables are complex, their perturbation expansion is simpler, because the zero-order values of  $W$  and  $Z$  are their initial conditions. Thus we find

$$\text{Im} \gamma_1 = -\frac{1}{2} \sin 2a \left[ \text{Re}(Z_1^{(1)}) - \text{Re}(e^{2ia} Z_1^{(2)}) \right],$$

where the argument of  $a$  is understood to be the excitation period  $\tau$ . The real part of  $\gamma_0$  is  $\sin^2 a \cos^2 a$ . When we insert the integrals, apply a trigonometric identity, and substitute into (3), we obtain the first-order shift

$$\delta\omega_1 = \frac{-4}{T \sin 2a} \left[ I_{CC} \cos a \sin \frac{1}{2} \Phi + I_{SS} \sin a \cos \frac{1}{2} \Phi \right] \cos \left( \frac{1}{2} \Phi + \varphi_p \right). \quad (4)$$

The integral  $I_{CC}$  is given by

$$I_{CC} = \int_0^\tau b_p(t) \cos \Omega(t - \tau/2) \cos[2a(t) - a(\tau)] dt.$$

The integral  $I_{SS}$  is the same except that both cosines are replaced with sines. This result is valid for excitations symmetric about their half-way point. For asymmetric excitation additional integrals are required. The integrals can be done analytically for constant excitation to yield the previously published result [6]. They can be easily done numerically for half-sine-wave excitation.

The first-order shift given by (4) has a sinusoidal dependence on the initial phase and a rapid oscillation with the sideband offset due to the phase advance  $\Phi$  between excitation regions. Figure 1 shows the envelope of this rapid oscillation for both constant and half-sine-wave excitation when the final cosine is replaced by unity.

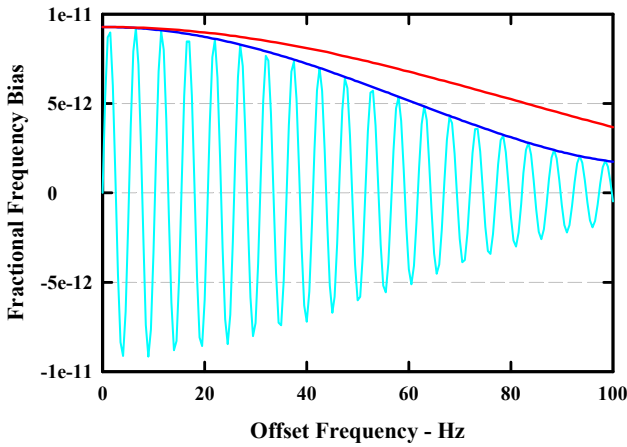


Figure 1. First-order sideband pulling. The light blue curve is for rectangular excitation. The dark blue curve is its upper envelope. The red curve is the envelope for half-sine-wave excitation.

## V. SECOND-ORDER SHIFTS

The second-order shift can be found in a similar, if more laborious, fashion. The imaginary part of  $\gamma_2$  has contributions from the second-order solution for  $Z$  and the product of first-order contributions from  $Z$  and  $W$ . These contributions involve the product of  $\cos\theta_a$  and  $\sin\theta_p$  at different times. A trigonometric identity allows this product to be written

$$2 \cos \theta_a(t) \sin \theta_p(t') = \sin(\Omega t + \Omega t' + \varphi_a + \varphi_p) - \sin(\Omega t - \Omega t' + \varphi_a - \varphi_p).$$

Therefore the second-order shift will depend only on the sum and difference of the initial phases and not on their individual values. When the computations are carried out, the shift from the second term in (3) has the form

$$\delta\omega_2 = \frac{b_a b_p}{T b^2} \left[ \begin{aligned} &Q_0 \cos(\varphi_a - \varphi_p) + (Q_C \cos \Phi + Q_S \sin \Phi) \cos \Theta \\ &+ (R_C \cos \Phi + R_S \sin \Phi) \cos(\varphi_a - \varphi_p) + R_0 \cos \Theta \end{aligned} \right],$$

where  $\Theta = \Phi + \Omega\tau + \varphi_a + \varphi_p$ . This shift is due to the combined action of phase and amplitude modulation. The coefficients are sums of integrals depending on  $a(\tau)$  and  $\Omega\tau$ , but of order unity. The  $Q$  coefficients arise from the interactions within each individual excitation region. The  $R$  coefficients arise from the interference between the first-order interactions in the two excitation regions. The terms with coefficients  $Q_C$ ,  $Q_S$ , and  $R_0$  do not contribute to the shift when the initial phases are averaged. But the remaining terms survive when  $\varphi_a - \varphi_p$  is constant. The  $Q_0$ ,  $R_C$ , and  $R_S$  coefficients are the ones computed for constant excitation by Audoin et. al. [4]. We have verified their results except that they did not include  $\tau$  in  $\Phi$ . The power dependence of their results was discussed in [5]. We note that these terms vanish if  $\varphi_a - \varphi_p = \pm\pi/2$ , the same condition that makes the two sidebands have equal intensity.

For atomic beam standards the last term in (3) vanishes, since the initial phase dependence in  $\text{Re}\gamma_1$  averages to zero. However, if this term is added in, as may be needed for pulsed standards, the  $Q$  coefficients are modified, but the  $R$  coefficients cancel out. Thus if the shift is then averaged over initial phases, only the  $Q_0$  term survives and there is no Ramsey-like oscillation in the shift. The modified  $Q_0$  term is plotted in figure 2 for both constant and half-sine-wave excitation.

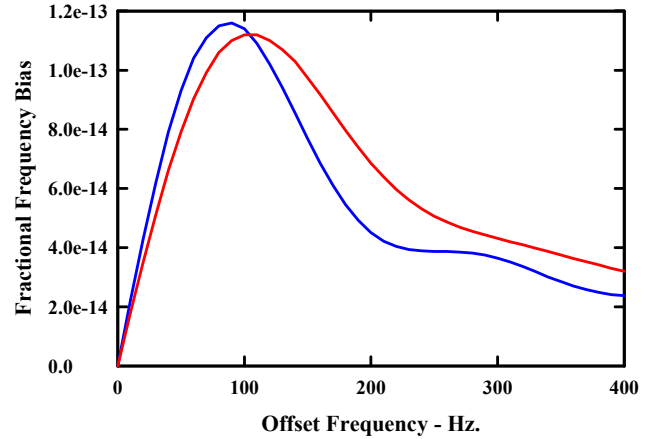


Figure 2. Second-order sideband pulling—initial phase-independent part. The blue curve is for constant excitation. The red curve is for half-sine-wave excitation.

## SUMMARY

We have theoretically studied sideband pulling in atomic frequency standards in terms of amplitude and phase modulation. We have introduced alternative variables to simplify a perturbation treatment of the modulation. We find the first-order pulling, generated by phase modulation, for both constant and half-sine-wave excitation. We find the second-order pulling is generated by the combined action of phase and amplitude modulation. We report the initial-phase and Ramsey-time dependence of the second-order shift.

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