Some Causes of Resonant Frequency Shifts in Atomic Beam Machines. II. The Effect of Slow Frequency Modulation on the Ramsey Line Shape

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Some Causes of Resonant Frequency Shifts in Atomic Beam Machines. II. The Effect of Slow Frequency Modulation on the Ramsey Line Shape

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The effect of slow frequency modulation of the exciting radiation on the Ramsey line shape observed in an atomic beam experiment is formulated theoretically. It is shown that the presence of second harmonic in the modulation can introduce measurable frequency shifts, whether observed directly or with a servo system.

1. INTRODUCTION

In attempting to build a clock based on the cesium resonance frequency, a servo system is often used to lock a crystal oscillator to the peak of the Ramsey line shape. The exciting radiation is frequency modulated at a slow rate, such that the instantaneous frequency sweeps across the center of the Ramsey line. The detector output then contains a component at the modulation frequency which vanishes when the excitation frequency coincides with a maximum (or minimum) of the Ramsey pattern.

A closer analysis of this situation shows that the concept of sweeping the excitation frequency across the line shape is physically erroneous unless the rate of sweep is extremely slow. If the frequency changes slightly during the time an atom is between the two oscillating field regions, the atom sees a phase shift upon entering the second oscillating field region. Such phase shifts produce quite different line shapes.[1] As the apparent phase shift oscillates with the modulation, the line shape oscillates among its various forms for the corresponding phase shifts. For sinusoidal modulation the line shape has a time dependence which is readily Fourier analyzed into components at multiples of the modulation frequency. The servo system looks only at the fundamental component of this series, adjusting the excitation frequency to minimize the amplitude of this component. Calculations indicate that this component vanishes at the Bohr frequency in the case of pure sinusoidal modulation. However, if harmonics are present in the modulation, the fundamental component may vanish at a slightly different frequency.

An approximate analysis is carried out to determine the effect on the Ramsey line shape of a slow, but otherwise arbitrary phase modulation. The results are applied to pure sine-wave modulation and then to modulation including a small amount of second harmonic.

2. ANALYSIS FOR ARBITRARY PHASE DEPENDENCE

The derivation of the line shape for unmodulated excitation has been discussed in a previous paper.[2] Reference should be made to Sec. 2 of that paper for the formulation and notation used. In the derivation of the Rabi line shape let us replace $\cos\omega t$ by $\cos[\omega t+\phi(t)]$. Carrying out the same procedure as in reference 2 we find the same expression for H_0, except that Δ has been replaced by

$$\Delta'=[\omega+\dot{\phi}(t)-\omega_0]/2.$$

This depends on time, but we now make the assumption that the change in $\dot{\phi}$ during the oscillating field region transit time τ is negligible compared with the Rabi linewidth. (In a typical case $\Delta\dot{\phi}/c$ is the order of 10^{-4} to 10^{-5}.) In the oscillating field regions we then treat $\dot{\phi}$ as constant, that is, $\dot{\phi}(t_0+\tau)=\dot{\phi}(t_0)$.

For Ramsey excitation we take the time dependence of ϕ into full account in the interim between the two oscillating field regions. In the first oscillating field region we use in the U matrix

$$\Delta_1=\Delta+\tfrac{1}{2}\dot{\phi}(t_0),$$

in the second,

$$\Delta_2=\Delta+\tfrac{1}{2}\dot{\phi}(t_0+T).$$

In between, ΔT is replaced by $\Delta T+\frac{1}{2}\delta\phi$, where $\delta\phi=\phi(t_0+T)-\phi(t_0)$ is the apparent phase shift for an atom entering at time t_0 and traversing the apparatus in time T. Combining the transformation matrices as in Sec. 4 of reference 2 the transition amplitude of the Ramsey pattern becomes

$$\beta=e^{i(\Delta T+\frac{1}{2}\delta\phi)}\alpha_0(\Delta_1)\beta_0(\Delta_2)+e^{-i(\Delta T+\frac{1}{2}\delta\phi)}\beta_0(\Delta_1)\bar{\alpha}_0(\Delta_2).$$

Written out in full this expression becomes somewhat unwieldy. Over the central peak of the Ramsey pattern, however, $\Delta\ll c$ whenever $\tau\ll T$ or $l\ll L$. To first order in Δ and $\dot{\phi}$

$$\begin{aligned}|\beta|^2=\tfrac{1}{2}\sin^2 2c\tau\{1+[&\cos2\Delta T-2(\Delta/c)\sin2\Delta T\tan c\tau]\\ &\times\cos\delta\phi-[\sin2\Delta T+2(\Delta/c)\cos2\Delta T\tan c\tau]\\ &\times\sin\delta\phi-(c^{-1}\sin2\Delta T\tan c\tau)\delta\omega\cos\delta\phi\\ &-(c^{-1}\cos2\Delta T\tan c\tau)\delta\omega\sin\delta\phi\},\end{aligned}$$

where $\delta\omega=\frac{1}{2}[\dot{\phi}(t_0)+\dot{\phi}(t_0+T)]$. Note that unless $\dot{\phi}^2$ terms are included the transition probability depends on ϕ only through the apparent phase shift $\delta\phi$ and the average frequency deviation $\delta\omega$. These depend on particle velocities through T, and on laboratory time through t_0.

If we observe the line shape over an extended period

[1] N. F. Ramsey, *Molecular Beams* (Oxford University Press, New York, 1956), p. 131.
[2] J. H. Shirley, J. Appl. Phys. 34, 783 (1963), preceding article.

of time, we see $|\beta|^2$ averaged over the entrance times of the atoms t_0. Let angular parentheses denote an average over t_0. The peak of the Ramsey pattern occurs at $\Delta_{\rm res}$, the root of $(d/d\Delta)|\beta|^2=0$. To the same approximation that $|\beta|^2$ was written

$$\tan 2\Delta_{\rm res}T = -\frac{\langle\sin\delta\phi\rangle+[2(\Delta_{\rm res}/c)\langle\cos\delta\phi\rangle+c^{-1}\langle\delta\omega\cos\delta\phi\rangle]\tan c\tau}{\langle\cos\delta\phi\rangle-[2(\Delta_{\rm res}/c)\sin\delta\phi+c^{-1}\langle\delta\omega\sin\delta\phi\rangle]\tan c\tau}.$$

If $\langle\sin\delta\phi\rangle$ and $\langle\delta\omega\cos\delta\phi\rangle$ both vanish, $\Delta_{\rm res}=0$ and there is no shift. If $\langle\sin\delta\phi\rangle\neq 0$, we have, neglecting terms of order $1/cT=O(l/L)$,

$$\tan 2\Delta_{\rm res}T=-\langle\sin\delta\phi\rangle/\langle\cos\delta\phi\rangle,$$

or for a small shift:

$$\omega_{\rm res}-\omega_0=-T^{-1}(\langle\sin\delta\phi\rangle/\langle\cos\delta\phi\rangle).$$

3. SIMPLE FREQUENCY MODULATION

Let us now consider the ideal case of pure sine-wave modulation

$$\phi=(b_1/\omega_m)\cos(\omega_m t+\delta_1).$$

Then

$$\delta\phi=-2(b_1/\omega_m)\sin(\tfrac{1}{2}\omega_m T)\times\sin(\omega_m t_0+\tfrac{1}{2}\omega_m T+\delta_1)=\delta\phi_1\sin W_1,$$

$$\delta\omega=-b_1\cos(\tfrac{1}{2}\omega_m T)\sin(\omega_m t_0+\tfrac{1}{2}\omega_m T+\delta_1)=\delta\omega_1\sin W_1.$$

We expand $\sin\delta\phi$ and $\cos\delta\phi$ in Fourier series in W_1, obtaining Bessel functions with argument $\delta\phi_1$ as coefficients[3]:

$$\sin\delta\phi=2J_1\sin W_1+2J_3\sin 3W_1+\cdots,$$
$$\cos\delta\phi=J_0+2J_2\sin 2W_1+2J_4\sin 4W_1+\cdots.$$

Now $\langle\sin nW_1\rangle=0$, so $\langle\sin\delta\phi\rangle=\langle\delta\omega\cos\delta\phi\rangle=0$ and no shift in the peak of the average line shape is expected.

We can go further and write out the Fourier expansion of $|\beta|^2$:

$$\begin{aligned}|\beta|^2=\tfrac{1}{2}\sin^2 2c\tau\Big\{&\Big[1+J_0\Big(\cos 2\Delta T-2\frac{\Delta}{c}\sin 2\Delta T\tan c\tau\Big)-J_1\frac{\delta\omega_1}{c}\Big]+\Big[-2J_1\Big(\sin 2\Delta T+2\frac{\Delta}{c}\cos 2\Delta T\tan c\tau\Big)\\&-J_0\frac{\delta\omega_1}{c}\sin 2\Delta T\tan c\tau\Big]\sin W_1\\&+\Big[-J_2\frac{\delta\omega_1}{c}\sin 2\Delta T\tan c\tau\Big]\cos W_1\\&+\Big[2J_2\Big(\cos 2\Delta T-2\frac{\Delta}{c}\sin 2\Delta T\tan c\tau\Big)\Big]\sin 2W_1\\&+\Big[(J_1-J_3)\frac{\delta\omega_1}{c}\cos 2\Delta T\tan c\tau\Big]\cos 2W_1+\cdots\Big\}\end{aligned}$$

[3] See, for example, Harold S. Black, *Modulation Theory* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1953), p. 188, or any work on Bessel functions.

We see that the constant term and the coefficients of even harmonics are even functions of Δ. They have maxima (or minima) at $\Delta=0$. The coefficients of the odd harmonics are odd functions of Δ, vanishing at $\Delta=0$. Thus a servo system which looks at the first harmonic and adjusts Δ to minimize the amplitude, seeks the desired resonance frequency. This is also true for modulation at several incommensurable frequencies, since they do not interfere with each other. For commensurable frequencies the situation is different.

4. EFFECT OF SECOND HARMONIC IN THE MODULATION

We take

$$\phi=(b_1/\omega_m)\cos(\omega_m t+\delta_1)+(b_2/2\omega_m)\cos(2\omega_m t+\delta_2)$$

and use the abbreviated notation

$$\delta\phi=\delta\phi_1\sin W_1+\delta\phi_2\sin W_2,$$
$$\delta\omega=\delta\omega_1\sin W_1+\delta\omega_2\sin W_2,$$

where

$$\delta\phi_k=-2(b_k/k\omega_m)\sin(\tfrac{1}{2}k\omega_m T),$$
$$\delta\omega_k=-b_k\cos(\tfrac{1}{2}k\omega_m T),$$

and

$$W_k=(k\omega_m t_0+\tfrac{1}{2}k\omega_m T+\delta_k).$$

For simplicity we consider $\delta\phi_2\ll 1$, with $\delta\phi_1$ arbitrary and keep only first-order terms in $\delta\phi_2$.

$$\sin\delta\phi=2J_1\sin W_1+2J_3\sin 3W_1-\delta\phi_2J_2\sin(2W_1-W_2)-\delta\phi_2J_0\sin W_2\cdots,$$

$$\cos\delta\phi=J_0+2J_2\cos 2W_1-\delta\phi_2J_1\cos(W_1-W_2)-\delta\phi_2J_3\cos(3W_1-W_2)+\cdots.$$

The argument of all Bessel functions is $\delta\phi_1$.

$$\langle\sin\delta\phi\rangle=\delta\phi_2J_2\sin(2\delta_1-\delta_2)\neq 0,$$

so a shift in the peak of the time-average line shape is expected, and will be approximately given by

$$\tan 2\Delta_{\rm res}T=\delta\phi_2(J_2/J_1)\sin(2\delta_1-\delta_2).$$

Neglecting terms which will be of order l/L

$$|\beta|^2=\tfrac{1}{2}\sin^2 c\tau(1+\cos 2\Delta T\cos\delta\phi-\sin 2\Delta T\sin\delta\phi).$$

The first harmonic of the detector output is then proportional to

$$\delta\phi_2[J_1\cos(W_1-W_2)+J_3\cos(3W_1-W_2)]\times\cos 2\Delta T+2J_1\sin W_1\sin 2\Delta T.$$

The mechanics of the servo system involve filtering out this frequency and feeding it into a phase detector. The output of the phase detector is proportional to the time average of the product of the input signal and a reference signal of the same frequency. Let the reference signal be proportional to $\sin(W_1+\theta)$. Then the phase detector output is proportional to

$$\delta\phi_2[J_1\sin(2\delta_1-\delta_2+\theta)-J_3\sin(2\delta_1-\delta_2-\theta)]\times\cos 2\Delta T+2J_1\cos\theta\sin 2\Delta T.$$

This is the correction signal to control the excitation frequency. The servo adjusts the excitation frequency so that the correction signal vanishes. This occurs when

$$\tan 2\Delta_{\text{res}}T=-\tfrac{1}{2}\delta\phi_2[(1-J_3/J_1)\sin(2\delta_1-\delta_2)+\tan\theta(1+J_3/J_1)\cos(2\delta_1-\delta_2)].$$

Thus the servo locks onto a frequency shifted from the Bohr frequency. The magnitude of the shift is in general *different* from the shift observed in the time-average line shape. It depends on the magnitude and relative phases of the modulating frequencies, and on the phase of the reference signal for the phase detector.

An analysis of the power spectrum of the modulated signal considered in this section shows an asymmetry proportional to $\sin(2\delta_1-\delta_2)$. If the relative phases of the modulating frequencies are such as to give a symmetric power spectrum *and if* the relative phase of the reference signal vanishes, there will be no shift. On the other hand, for $\theta=\pi/2$, the shift can be sizeable (about 10^{-9} for cesium), so that it is desirable to observe the "in phase" component of the detector signal as well as to have symmetric power spectra in order to keep the shifts small. For $\delta\phi_1=O1$, $\delta\phi_2=O10^{-2}$, $\theta=0$, $T=O10^{-2}$,

$$(\omega_{\text{res}}-\omega_0)/\omega_0=2\Delta/\omega_0=O(\delta\phi_2/2\omega_0T)=O10^{-11}$$

for cesium. This estimate shows that the shift due to second harmonic in the modulation can be appreciable unless the amplitude of the second harmonic is kept very small. (Shifts due to the second harmonic have been observed and the dependence on the amplitudes and relative phases plotted by the National Company in their research on cesium beam frequency standards.[4] Unfortunately they did not present their theoretical work on the problem.)

The inclusion of higher harmonics only complicates the analysis. However, the odd harmonics alone do not produce any shifts. The general formula for the shift is always a sum of products of even and odd harmonics.

5. EFFECT OF VELOCITY DISTRIBUTION

In the preceding analysis no mention has been made of the velocity distribution and, in fact, no attempt has been made to average over velocities. We note that not only $\tan 2\Delta T$ and $\sin^2 c\tau$ depend on velocity, but also $\delta\phi_1$ and $\delta\phi_2$, hence all Bessel functions, also $\delta\omega_1$, $\delta\omega_2$, and θ (to compensate for T dependence in W_1). Ramsey's tables (reference 1, p. 423) do not include integrals of the form

$$\int_0^\infty e^{-y^2}y^3\sin\left(\frac{x}{y}\right)J_n\left(a\sin\frac{b}{y}\right)dy.$$

Qualitatively the results of this paper should not be changed appreciably by a velocity average from what they are using a single median velocity. If more than a rough value for the size of the shift were desired a numerical averaging would have to be performed to find a numerical magnitude for the shift. But because of the velocity distribution it is impossible to eliminate the shift simply by adjusting $\theta=0$ or $\delta\phi_1$ such that $J_1=J_3$, since these could hold only for a single velocity. However, since the sign of the shift can reverse, there must still exist conditions for which the shift seen by the servo, or the shift in the time-average line shape (but not both) vanishes. It would be difficult to compute these conditions theoretically, especially since they will depend sensitively on the power level of the excitation. But it should be possible by trying for a symmetric power spectrum and $\theta\approx 0$ to reduce the shift by one or two orders of magnitude below the estimate made in Sec. 4.

A change in excitation power level (c^2) changes the velocity for which the transition probability is a maximum, hence changes the relative effectiveness of the velocity components of the beam. Any velocity-dependent shift such as the one found in Sec. 4 then exhibits a marked and complex dependence on power level, and it is difficult to separate such shifts according to their causes.

[4] Interim Development Report for Atomic Beam Frequency Standard, 4-28-57 to 7-27-57, National Company, Inc., Malden, Massachusetts (1957).