WEIGHT FUNCTIONS FOR BIASES IN ATOMIC FREQUENCY STANDARDS*

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We present a unified treatment of frequency-standard biases that vary significantly during the period of measurement. We introduce three time-dependent weight functions built from the solution of the unperturbed equations of motion for a two-level system. By integrating a weight function together with the time dependence of a perturbation over the excitation period we find the change in the lineshape and can deduce any biases. The same weight function may be used for treating more than one cause of a bias.

1. Introduction of weight functions

We summarize a formulation based on the time-dependent Schrödinger equation as presented in [1]. A corresponding analysis may also be done by use of the three-component equations derived from the density matrix [2, 3].

The Hamiltonian for a two-level system excited by radiation at frequency ω can be written $\mathcal{H} = -\Delta\sigma_z + b\sigma_x$, where the σ_i are the Pauli spin matrices. We have introduced the abbreviation $\Delta = \frac{1}{2}(\omega - \omega_0)$ for one half the detuning from the atomic resonance frequency ω_0. Similarly, b is one half the Rabi frequency associated with the excitation. The coefficients b and Δ are both real and may be time-dependent. We have applied the rotating-wave approximation and redefined the phases of the wave-function components to eliminate the rapid time dependence of the coupling coefficient b [1].

The components α and β of the wave function obey the time-dependent Schrödinger equation,

$$\begin{aligned} i d\alpha/dt &= -\Delta\alpha + b\beta \\ i d\beta/dt &= b\alpha + \Delta\beta \end{aligned}, \qquad (1)$$

with the initial conditions $\alpha(0) = 1$ and $\beta(0) = 0$. The probability that a transition has occurred after excitation for a period τ is then $P = |\beta(t)|^2$.

A two-level perturbation Hamiltonian can be represented by $\mathcal{H}_1 = \hbar \sum_i G_i(t)\sigma_i$, where the index i ranges over x, y, z and the $G_i(t)$ are real. The x component of the sum represents a perturbation in the amplitude of the exciting field. The y component represents a perturbation in the phase of the exciting field. The z component represents a perturbation in either the frequency of the exciting field or the energy-level separation.

The presence of a perturbation alters the wave function by ψ_1, which satisfies $i\hbar\frac{d}{dt}\psi_1 = \mathcal{H}\psi_1 + \mathcal{H}_1\psi$ to first order in the perturbation. A formal solution to this equation at time τ is

$$\psi_1(\tau) = -(i/\hbar)U(\tau,0)\int_0^{\tau} U^{-1}(t,0)\mathcal{H}_1(t)\psi(t)\,dt\,,$$

where $U(t,0)$ is the evolution matrix for the unperturbed system. The wave function correction ψ_1 is thus expressed as an integral over the time dependence of the perturbation with functions known from the solution of the unperturbed Schrödinger equation.

To first order the correction to the transition probability is also an integral over the perturbation with a function built up from solutions of (1):

$$P_1(\tau) = \int_0^{\tau}\sum_i W_i(\tau,t)G_i(t)dt\,. \qquad (2)$$

We call the real functions $W_i(\tau,t)$ weight functions, because they weight the averaging of the perturbation time dependence. Each weight function depends on intermediate and final times, as well as the unperturbed excitation amplitude b and detuning Δ. Each weight function can be expressed in terms of the unperturbed probability amplitudes α and β satisfying (1) as follows:

Amplitude weight function: $$W_x(\tau,t) = \mathrm{Im}\left\{2\alpha(\tau)^*\beta(\tau)^*\left[\alpha(t)^2 - \beta(t)^2\right]\right\} \qquad (3)$$

Phase weight function: $$W_y(\tau,t) = \mathrm{Re}\left\{2\alpha(\tau)^*\beta(\tau)^*\left[\alpha(t)^2 + \beta(t)^2\right]\right\} \qquad (4)$$

Detuning weight function: $$W_z(\tau,t) = -\mathrm{Im}\left[4\alpha(\tau)^*\beta(\tau)^*\alpha(t)\beta(t)\right]. \qquad (5)$$

The detuning weight function is equivalent to the sensitivity function used in analysis of the Dick effect [3,4].

In figure 1 we plot the three weight functions as a function of t for half-sine-wave Rabi excitation $b(t) = (\pi/2)b_0\sin(\pi t/\tau)$. These functions were found by inserting numerical solutions of (1) for α and β into (3)-(5).

1.1. *Properties of Weight Functions*

From the symmetries of the real and imaginary parts of α and β, we find that W_x is an even function of the detuning Δ, while W_y and W_z are odd functions. Thus an amplitude perturbation adds a symmetric contribution to the lineshape but does not shift the resonance frequency. Phase and detuning perturbations add asymmetric contributions to the lineshape and may shift the resonance frequency.

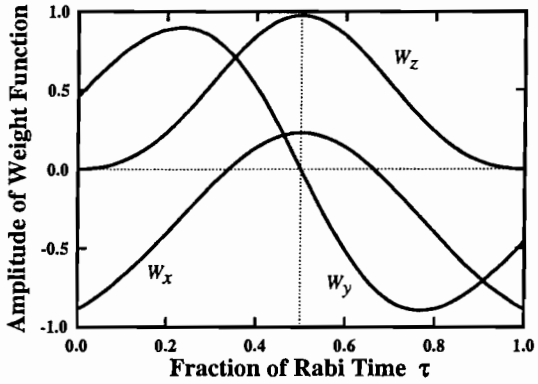

Fig. 1. Weight functions for Rabi excitation evaluated at $b_0\tau = 0.50\pi$ (optimum excitation) and $\Delta\tau = 0.544\pi$ (halfwidth of the Rabi lineshape).

From the time symmetry of the unperturbed Schrödinger equation we find that if the unperturbed excitation amplitude $b(t)$ is symmetric about the mid-excitation time $\tau/2$, then W_x and W_z are symmetric about $\tau/2$, while W_y is anti-symmetric. Conversely, if $b(t)$ is antisymmetric about time $\tau/2$, then W_y and W_z are symmetric about $\tau/2$, while W_x is antisymmetric. These symmetries combine with the time symmetries of perturbations to null certain effects.

1.2. *Relations of weight functions*

From (1) and the definitions (3)-(5) we deduce that the weight functions obey the following differential equations:

$$\begin{aligned} \partial W_x / \partial t &= 2\Delta W_y \\ \partial W_y / \partial t &= -2\Delta W_x - 2bW_z \\ \partial W_z / \partial t &= 2bW_y \end{aligned} .$$

These equations have the same form as the three-component equations [2,3], but have different initial conditions.

2. Biases in Rabi excitation

Consider slow square-wave modulation of the exciting frequency with amplitude ω_m. We define the resonance position by that detuning $\delta\omega$ that makes the signals at the detunings $\omega_m+\delta\omega$ and $-\omega_m+\delta\omega$ equal. To first order, this resonance position becomes $\delta\omega = -P_1(\omega_m)/\partial P(\omega_m)/\partial\omega$. To obtain a bias, we compute the numerator from (2) and the denominator from the unperturbed lineshape.

Suppose the atomic resonance frequency varies during the period of excitation. The z-component of (2) tells us how to average the variation. Figure 1 shows that the detuning weight function emphasizes the mid-time part of the variation. Any asymmetric part of the variation averages to zero.

As an example of a phase perturbation, consider phase modulation at frequency Ω with half Rabi amplitude b_1 and initial phase φ. It can be represented by the perturbation function $G_y = b_1 \sin(\Omega t + \varphi)$. If we add and subtract $\frac{1}{2}\Omega\tau$ to the argument of the sine we can rewrite it as follows:

$$\sin(\Omega t + \varphi) = \sin\Omega\left(t - \tfrac{1}{2}\tau\right)\cos\left(\tfrac{1}{2}\Omega\tau + \varphi\right) + \cos\Omega\left(t - \tfrac{1}{2}\tau\right)\sin\left(\tfrac{1}{2}\Omega\tau + \varphi\right).$$

For excitations symmetric about $t = \frac{1}{2}\tau$, the phase weight function W_y is anti-symmetric. The second term is symmetric, hence its integral with W_y vanishes. The factor $\cos\left(\frac{1}{2}\Omega\tau + \varphi\right)$ in the first term is independent of t, hence may be removed from the integral. The change in lineshape reduces to

$$P_1 = \int_0^\tau W_y(\tau, t)\, b_1 \sin\Omega\left(t - \tfrac{1}{2}\tau\right) dt \cos\left(\tfrac{1}{2}\Omega\tau + \varphi\right).$$

The final cosine factor completely describes the dependence of P_1 and the corresponding shift on the initial phase. As discussed in [5] any thorough average over φ eliminates this first order shift. For constant excitation we can perform the integration. The result agrees with that given in (7) of [5].

3. Biases in Ramsey excitation

Ramsey excitation consists of two short periods of excitation separated by a relatively long "drift" period T free of excitation. Weight functions for Ramsey excitation are still defined by (3)-(5), but the probability amplitudes now refer to the complete cycle spanning both excitations. The integral (2) must span both excitations. The symmetries of the weight functions are the same as given before. But note that time symmetry is now about the midpoint of the drift time.

Figure 2 shows the shape of the three weight functions as a function of time for T = 4τ and 2 dB below optimum excitation. All of W_x and the central part of W_y vanish when the excitation is exactly optimum.

Consider first that the atomic resonance ω_0 is changing, as it might in an inhomogeneous magnetic field. During the drift time, Fig. 2 shows that W_z is constant. Hence the unweighted time average of ω_0 is adequate . Changes in ω_0 during excitation are underweighted toward the beginning of the first excitation and the end of the second excitation.

The following four causes of frequency biases can all be interpreted as perturbations of phase and all treated using the *same* weight function G_y: end-to-end cavity phase shift, microwave leakage, distributed cavity phase shift and

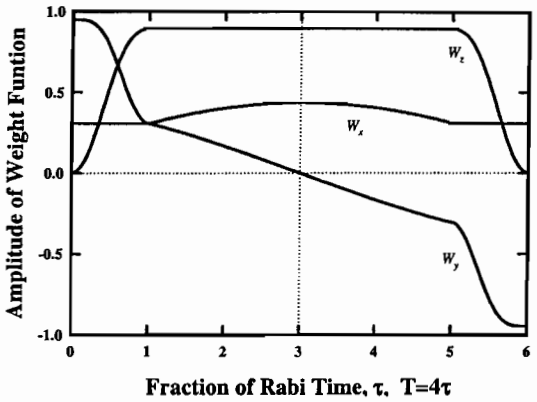

Fig. 2. Weight functions for Ramsey excitation evaluated at $2b_0\tau = 0.40\pi$ and $2\Delta T = .50\pi$ (halfwidth of a Ramsey fringe).

sidebands or spurs on the exciting radiation. They differ in the regions over which the integral in (2) is zero.

For example, the perturbation effect of phase modulation is found by use of the same perturbation function, as in the Rabi case. But the integration now extends over both excitation regions. For symmetric excitation about the mid-time $t = \frac{1}{2}T + \tau$, we can factor out the initial phase dependence, just as we did in the Rabi case. We then find the perturbation transition probability

$$P_1 = 2\int_0^{\tau} W_y(\tau, t)\sin\Omega\left(t - \tau - \tfrac{1}{2}T\right)dt\cos\left(\tfrac{1}{2}\Omega T + \Omega\tau + \varphi\right).$$

The symmetry of the integrand assures us that the integration result is the same for both excitation regions. For constant excitation the integral can be evaluated. The result is in agreement with (15) in [5], but the derivation here is much shorter.

A more detailed paper with additional examples is planned for publication elsewhere.

References

1. J. H. Shirley, W. D. Lee, R. E. Drullinger, *Metrologia* **38**, 427-458 (2001).
2. J. Vanier and C. Audoin, *The Quantum Physics of Atomic Frequency Standards* (Adam Hilger, Ed., IOP Publishing Ltd., Bristol, England, 1989).
3. P. Lemonde, G. Santarelli, Ph.Laurent, F. P. Dos Santos, A. Clairon, C. Salomon, *Proc. IEEE Int. Freq. Control Symp.*, 110-115 (1998).
4. G. J. Dick, *Proc. 19th PTTI*, 133-147 (1987).
5. J. H. Shirley, T. P. Heavner, S. R. Jefferts, to appear in *IEEE Trans. Inst. Meas.*