Weight Functions for Biases in Atomic Frequency Standards

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***Abstract*—Many perturbations that affect atomic frequency standards vary during the period of measurement. To include this time variation, we introduce 3 time-dependent weight functions built from the solution of the unperturbed equations of motion of a 2-level system. The integral of the time-dependent part of a perturbation with a weight function gives the associated first-order change in transition probability. Biases are then found easily. The same weight function may be used for different perturbations, thus unifying the derivation of their associated biases. We give several examples of the use of weight functions.**

I. Introduction

Several biases affect the frequencies of primary frequency standards. Some of these (black-body, gravitational red shift) are nearly constant throughout a measurement. These biases may be treated independently of the method of measurement. Other biases (magnetic field) may have small spatial variations that moving atoms see as time variations. Still other biases (e.g., due to leakage of the excitation field, distributed cavity phase variation, second-order Doppler effect in fountains) may vary considerably during the measurement period. In the past, specific theories have been developed to treat each individual source of bias. Only a few publications collect these theories together [1]–[3].

In this paper, we present a formalism that permits a unified treatment of biases that vary significantly during the period of measurement. We introduce 3 time-dependent weight functions built from the solution of the unperturbed equations of motion. These functions describe the first-order response of the atomic transition probability to time-dependent perturbations. By integrating a weight function together with the time dependence of a perturbation over the measurement period, we find the change in the line shape and can deduce any associated biases. These weight functions incorporate the parameters that depend on the method of measurement. The advantage of using weight functions is that much of the algebra involved in solving the perturbed equations of motion, extracting the transition amplitude, and constructing the transition probability is done once and need not be repeated for different perturbations. An abbreviated version of this work has appeared previously [4].

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In Section II, we present the Schrödinger equation of motion for a 2-level system with a small perturbation. We then derive the weight functions and discuss their properties. In Section III, we apply the weight functions to Rabi (single zone) excitation to find the distortions of the line shape due to a perturbation. In Section IV, we present weight functions for Ramsey (dual zone) excitation. From them we derive several shifts relevant to primary frequency standards. Section V summarizes our results. The appendix shows the equivalence of our detuning weight function to the sensitivity function employed in analysis of the Dick effect [5].

II. Derivation of Weight Functions

We present here a formulation based on the time-dependent Schrödinger equation for a 2-level system as presented in [3]. A corresponding analysis may also be carried out by use of the 3-component equations derived from the density matrix [2], [6], [7].

A. Unperturbed Equations of Motion

The time-dependent Schrödinger equation for a 2-level system excited by radiation at frequency ω can be written as

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi_{\mathrm{S}} = \mathcal{H}_{\mathrm{S}}\psi_{\mathrm{S}}, \tag{1}$$

with $\psi_{\mathrm{S}} = \begin{pmatrix} C_a \\ C_b \end{pmatrix}$ and

$$\mathcal{H}_{\mathrm{S}} = \hbar \begin{pmatrix} \omega_a & 2b\cos(\omega t + \theta) \\ 2b\cos(\omega t + \theta) & \omega_b \end{pmatrix}.$$

Here ψ_{S} is the 2-component wave function, $\mathcal{H}_{\mathrm{S}}$ is the Hamiltonian, and $\hbar\omega_a$ and $\hbar\omega_b$ are the energies of the upper and lower states. The amplitude of the excitation is denoted by the Rabi frequency $2b$; θ is the phase of the applied field at $t = 0$. Both b and θ are real and may vary with time, but slowly compared with ωt.

The first step in solving (1) is the rotating wave approximation. We write the cosine in the interaction term as the sum of 2 exponentials. We then keep only the exponential that "rotates" in the same sense as the "precession" corresponding to the energy levels, where the terms in quotes have physical meaning for magnetic resonance of a spin-one-half system [6]. That is, we replace the Hamiltonian by

$$\mathcal{H}_{\rm rot} = \hbar \begin{pmatrix} \omega_a & be^{-i\omega t}e^{-i\theta} \\ be^{i\omega t}e^{i\theta} & \omega_b \end{pmatrix}$$

when $\omega_a > \omega_b$. The principal correction caused by the "anti-rotating" part of the Hamiltonian is the Bloch-Siegert bias [3], [8]–[10].

The second step in solving (1) is to define new probability amplitudes that differ from C_a and C_b by time-dependent phases:

$$\alpha(t) = C_a(t)\exp[i\phi_a(t)] \quad \text{and} \quad \beta(t) = C_b(t)\exp[i\phi_b(t)].$$

The new amplitudes α and β are the components of a wave function ψ obeying

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi = \mathcal{H}\psi. \tag{2}$$

By choosing the phase changes

$$\begin{aligned} \phi_a &= (\omega + \omega_a + \omega_b)t/2 + \theta/2 \quad \text{and} \\ \phi_b &= (-\omega + \omega_a + \omega_b)t/2 - \theta/2, \end{aligned}$$

the new unperturbed Hamiltonian becomes

$$\mathcal{H} = \hbar \begin{pmatrix} -\Delta & b \\ b & \Delta \end{pmatrix},$$

where the coefficients b and Δ are both real. We have introduced the abbreviation $\Delta = (1/2)\ (\omega - \omega_0)$ for one-half the detuning from the atomic resonance frequency $\omega_0 = \omega_a - \omega_b$. Similarly, b is one-half the Rabi frequency associated with the excitation. We have here assumed θ constant, but either or both of b and Δ may be time dependent. With these phase changes, we have eliminated the rapid time dependence and complex phase of the coupling coefficients b. We have also made the new Hamiltonian real and traceless.

In component form, the time-dependent Schrödinger equation (2) with the new Hamiltonian becomes

$$\begin{aligned} i\mathrm{d}\alpha/\mathrm{d}t &= -\Delta\alpha + b\beta \\ i\mathrm{d}\beta/\mathrm{d}t &= b\alpha + \Delta\beta. \end{aligned} \tag{3}$$

We further define α and β as those solutions of (3) obeying the initial conditions $\alpha(0) = 1$ and $\beta(0) = 0$. The probability that a transition has occurred after excitation for a time τ is then represented by

$$P(\tau) = \left|\beta(\tau)\right|^2.$$

The form of (2) or (3) guarantees that the normalization of the wave function is constant at all times

$$\left|\alpha(t)\right|^2 + \left|\beta(t)\right|^2 = 1.$$

In general, the solution of (3) cannot be found analytically when either b or Δ is time-dependent.

If we write out the real and imaginary parts of the 2 equations in (3)—compare [11, eq. (4)]—we have 4 coupled equations in 4 real variables. When the initial conditions hold, we see that Reα and Imβ are even functions of the detuning Δ, while Imα and Reβ are odd functions. The transition probability, which is the sum of the squares of the real and imaginary parts of β, is thus an even function of detuning and hence centered on the resonance. This remains true independent of any time variation that b may have.

The general solution of (2) can be expressed by

$$\psi(t) = U(t,0)\psi(0),$$

where the unitary evolution matrix $U(t,0)$ satisfies (2) and the initial condition that $U(0,0)$ is the unit matrix. For our 2-level system, the evolution matrix must have the form

$$U(t,0) = \begin{pmatrix} \alpha(t) & -\beta^*(t) \\ \beta(t) & \alpha^*(t) \end{pmatrix}.$$

Thus the probability amplitudes when the system starts from one state are trivially related to those when the system starts from the other state (change the sign of the detuning Δ).

B. Perturbation Hamiltonian

A 2-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 σ_i are the Pauli spin matrices. The perturbation functions $G_i(t)$ are real to preserve hermiticity of the Hamiltonian. 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. Note that here and in the following, quantities without subscript refer to the unperturbed Hamiltonian and wave function, while quantities with subscript 1 refer to first-order corrections due to a perturbation.

In the presence of the perturbation Hamiltonian, the wave function is altered by ψ_1, which satisfies

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\psi_1 = \mathcal{H}\psi_1 + \mathcal{H}_1\psi$$

to first order in the perturbation. A formal solution to this equation at time τ is

$$\psi_1(\tau) = -(i/\hbar)U(\tau,0)\int_0^\tau U^{-1}(t,0)\mathcal{H}_1(t)\psi(t)\,\mathrm{d}t. \tag{4}$$

The perturbation correction ψ_1 is thus expressed as an integral over the time dependence of the perturbation weighted by functions known from the solution of the unperturbed Schrödinger equation (3).

C. Definition of Weight Functions

The first-order perturbation correction to the transition probability is

$$P_1(\tau) = 2\,\mathrm{Re}\left[\beta^*(\tau)\beta_1(\tau)\right], \tag{5}$$

where the transition amplitude perturbation β_1 can be extracted from the wave function in (4). To first order, the correction to the transition probability is thus also an integral over the perturbation time dependence. We write it as

$$P_1(\tau) = \int_0^\tau \sum\nolimits_i W_i(\tau,t) G_i(t)\,\mathrm{d}t. \tag{6}$$

We have substituted the expression for $\mathcal{H}_1$ in terms of the $G_i(t)$ into (4). We then extracted $\beta_1(\tau)$ from $\psi_1(\tau)$, inserted it into (5), and combined $\beta^*(\tau)$ with all the other unperturbed quantities from the evolution matrices into the coefficients $W_i(\tau,t)$ of the $G_i(t)$. We call the resulting real functions $W_i(\tau,t)$ weight functions, because they weight the averaging of the perturbation time-dependence implied by the integral. Each weight function depends on intermediate and final times, as well as the unperturbed excitation amplitude and detuning.

The weight functions can be expressed in terms of the unperturbed transition amplitudes α and β. When we carry out the matrix multiplications in (4) we find the definitions

$$W_x(\tau,t) = \mathrm{Im}\left\{2\alpha(\tau)^*\beta(\tau)^*\left[\alpha(t)^2 - \beta(t)^2\right]\right\}, \tag{7}$$

$$W_y(\tau,t) = \mathrm{Re}\left\{2\alpha(\tau)^*\beta(\tau)^*\left[\alpha(t)^2 + \beta(t)^2\right]\right\}, \tag{8}$$

and

$$W_z(\tau,t) = -\mathrm{Im}\left[4\alpha(\tau)^*\beta(\tau)^*\alpha(t)\beta(t)\right]. \tag{9}$$

In deriving these definitions, several terms in β_1 have been dropped, because they do not contribute to the real part in (5). In accordance with the nature of the perturbation, we refer to W_x as the amplitude weight function, W_y as the phase weight function, and W_z as the detuning weight function. Other equivalent ways of writing these definitions may be found, for example, in terms of α and β with argument τ-t.

D. Properties of Weight Functions

1) Detuning Symmetry: If we insert the symmetries of the real and imaginary parts of α and β into the definitions of the weight functions, 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 line shape but does not shift the resonance. Phase and detuning perturbations contribute asymmetrically to the line shape and may shift the resonance.

2) Time Symmetry: From the time symmetry of the unperturbed Schrödinger equation, one can show 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 antisymmetric. 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 can combine with the time symmetries of perturbations to null certain effects.

3) Values at End Points: From the initial conditions on α and β, we find the following initial values of the weight functions:

$$\begin{aligned} W_x(\tau,0) &= \mathrm{Im}\left[2\alpha(\tau)^*\beta(\tau)^*\right] \\ W_y(\tau,0) &= \mathrm{Re}\left[2\alpha(\tau)^*\beta(\tau)^*\right] \\ W_z(\tau,0) &= 0. \end{aligned} \tag{10}$$

Similarly, the final values of the weight functions are

$$\begin{aligned} W_x(\tau,\tau) &= \mathrm{Im}\left[2\alpha(\tau)\beta(\tau)^*\right] \\ W_y(\tau,\tau) &= \mathrm{Re}\left[2\alpha(\tau)\beta(\tau)^*\right] \\ W_z(\tau,\tau) &= 0. \end{aligned} \tag{11}$$

E. Relations of Weight Functions

The 3 weight functions are closely related to each other. From (3) and the definitions (7)–(9), we deduce that the weight functions obey the following differential equations:

$$\begin{aligned} \partial W_x/\partial t &= 2\Delta W_y \\ \partial W_y/\partial t &= -2\Delta W_x - 2b W_z \\ \partial W_z/\partial t &= 2b W_y. \end{aligned} \tag{12}$$

These equations have the same form as the 3-component equations of motion [2], [7], but may have different initial conditions. From these equations plus (10) and (11), we can determine the initial and final slopes of the weight functions. For example,

$$\partial W_z(\tau,0)/\partial t = 2b(0)\,\mathrm{Re}\left[2\alpha(\tau)^*\beta(\tau)^*\right] \quad \text{and}$$
$$\partial W_z(\tau,\tau)/\partial t = 2b(\tau)\,\mathrm{Re}\left[2\alpha(\tau)\beta(\tau)^*\right].$$

Hence, the initial and final slopes of the detuning weight function depend on the initial and final values of the excitation.

F. Weight Functions for Constant Excitation

When b and Δ are constant, an analytic solution of (3) can be found:

$$\alpha(t) = \cos pt + i(\Delta/p)\sin pt \quad \text{and} \quad \beta(t) = -i(b/p)\sin pt,$$

where $p^2 = b^2 + \Delta^2$. When inserted into (7)–(9), the weight functions can be expressed as

$$W_x(\tau,t) = \frac{b^3}{p^3}\sin 2p\tau + \frac{2b\Delta^2}{p^3}\sin p\tau \cos p(\tau - 2t),$$

$$W_y(\tau,t) = \frac{2b\Delta}{p^2}\sin p\tau \sin p(\tau - 2t),$$

and

$$W_z(\tau,t) = -\frac{2b^2\Delta}{p^3}\sin p\tau\left[\cos p\tau - \cos p(\tau - 2t)\right].$$

These expressions obey the symmetries just described. They also obey the differential equations (12).

In Figs. 1(a)–(c), we plot the 3 weight functions for constant excitation as a function of t with $b\tau = 0.50\pi$ (optimum power) and $\Delta\tau = 0.40\pi$ (half width of the Rabi line shape). Also plotted are the same weight functions for half-sine-wave excitation $b(t) = (\pi/2)b_0\sin(\pi t/\tau)$ for $b_0\tau = 0.50\pi$ (optimum power) and $\Delta\tau = 0.544\pi$ (half width of the Rabi line shape). The latter functions were found by inserting numerical solutions of (3) into (7)–(9). Note the change in the initial and final slopes of the detuning weight function with the change in the form of excitation.

G. Conversion Between Phase and Detuning Perturbations

Phase and detuning perturbations are closely related. Consider a small, time-dependent phase perturbation θ_1 added to the constant phase θ. The Hamiltonian then has the off-diagonal elements $b\exp(i\theta_1) \approx b + ib\theta_1$ and its complex conjugate. The imaginary part is the phase perturbation. It causes a line-shape perturbation given by (6):

$$P_1 = \int_0^\tau W_y(\tau,t)b(t)\theta_1(t)\,\mathrm{d}t.$$

From the last relation of (12), we can replace bW_y by half the derivative of W_z. An integration by parts then leads to

$$P_1 = -\frac{1}{2}\int_0^\tau W_z(\tau,t)(\mathrm{d}\theta_1/\mathrm{d}t)\,\mathrm{d}t, \qquad (13)$$

because W_z vanishes at both endpoints by (10) and (11). Thus, we have re-expressed the phase perturbation as a detuning perturbation. If we had included θ_1 with θ in our phase factoring, half its time derivative would have appeared along with Δ in our original Hamiltonian. We could have interpreted this appearance of $\mathrm{d}\theta_1/\mathrm{d}t$ as a variation of the detuning. Thus, we have 2 equivalent ways of treating phase perturbations. This equivalence has already been noted by Lemonde *et al.* [7].

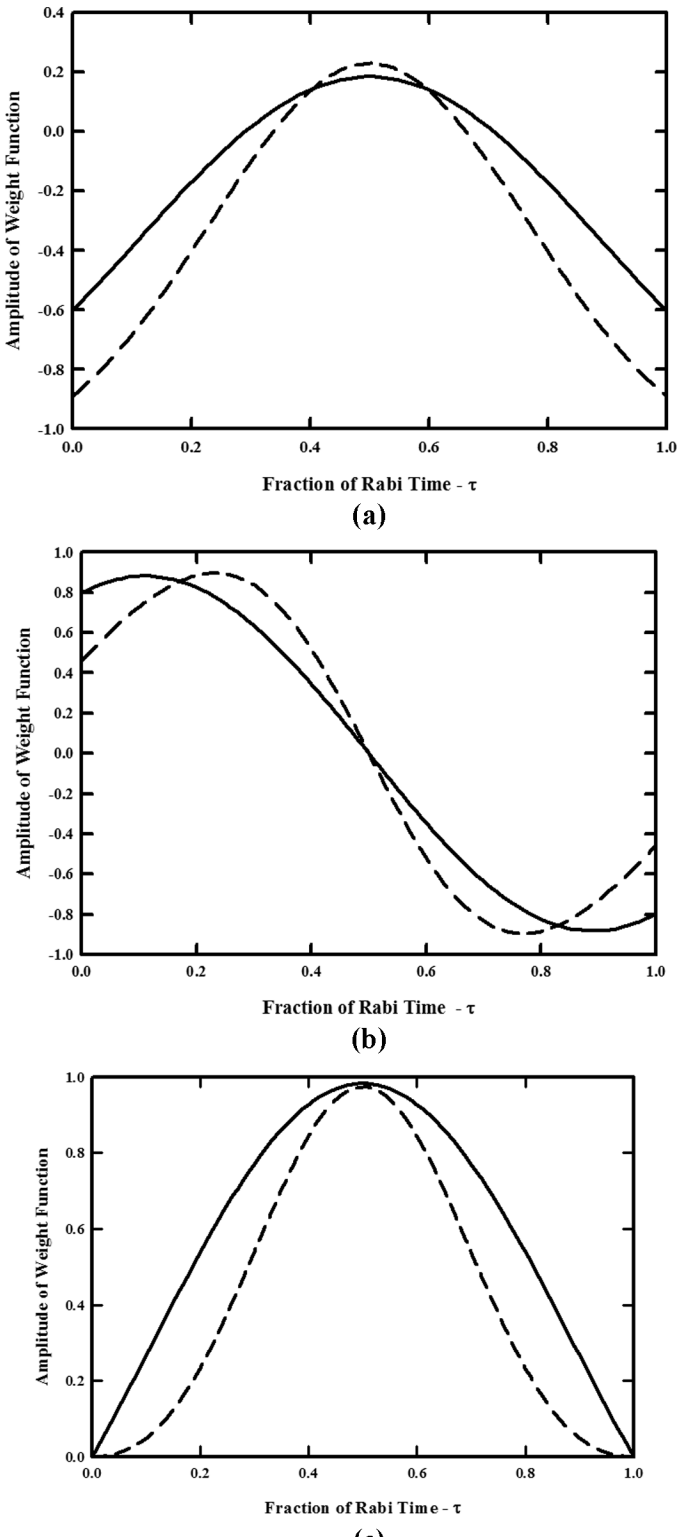

Fig. 1. Weight functions for Rabi excitation evaluated at optimum power and half-width detuning. The solid line is for constant excitation amplitude. The dashed line is for half-sine-wave excitation. (a) Amplitude weight function, (b) phase weight function, and (c) detuning weight function.

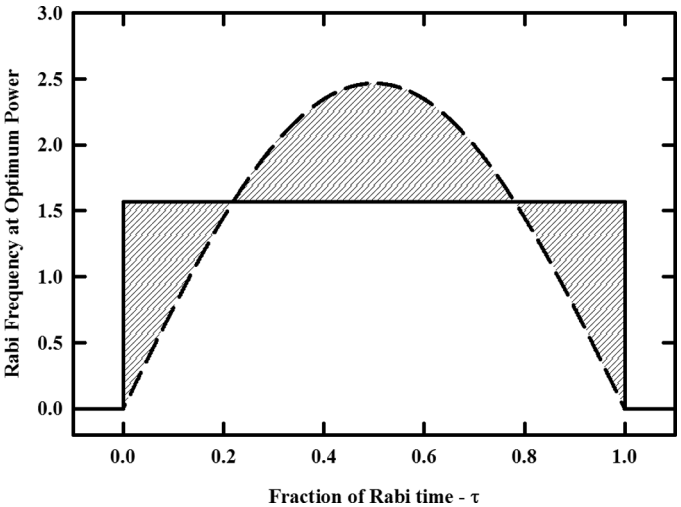

Fig. 2. Comparison of constant (solid line) and half-sine-wave (dashed line) excitation amplitudes enclosing the same area. The difference between these (shaded areas) was treated as a perturbation.

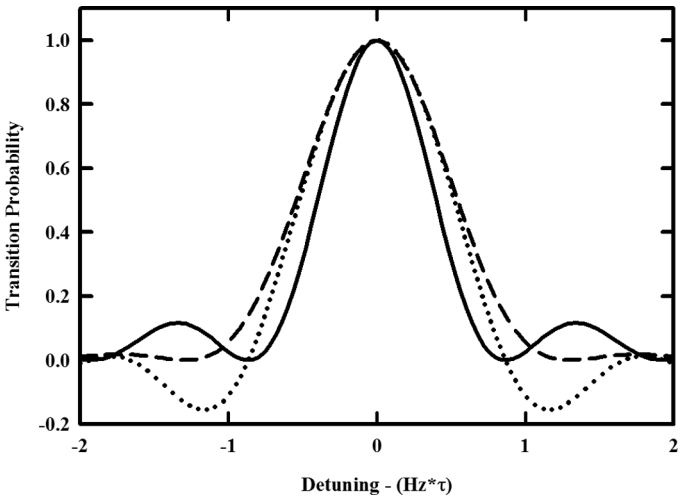

Fig. 3. Comparison of Rabi line shapes for different excitation amplitude time dependences. The solid line is for constant excitation. The dotted line is for constant excitation with a first-order correction to simulate half-sine-wave excitation. The dashed line is exact for half-sine-wave excitation.

III. Perturbations in Rabi Excitation

Following are examples of the use of each weight function for analyzing some perturbations occurring in single zone or Rabi excitation.

A. Variation of Excitation Amplitude

1) Asymmetry: The excitation amplitude $b(t)$ may be nearly, but not perfectly, symmetric about $\tau/2$. Asymmetry could exist if, for example, the losses are unequal at the entrance and exit planes of the microwave cavity enclosing the exciting field. Also, if the atoms are interrogated during vertical flight, as in fountains, the gravitational slowing of the atoms will cause them to perceive an asymmetry in time even when the spatial dependence is symmetric. For symmetric excitation, the amplitude weight function is symmetric. The integral (6) of a small asymmetric part of $b(t)$ then vanishes. Thus, there is no first-order change in the line shape.

2) Line Shapes for Half-Sine-Wave Excitation Versus Constant Excitation: Many primary frequency standards use a cavity mode such that the atoms see a half-sine-wave excitation amplitude. But no analytic solution of (3) is available for this case. Fig. 2 shows the difference in $b(t)$ between half-sine-wave and constant excitation, scaled so they each enclose the same area. Although the difference is not very small, we have treated it as a perturbation to obtain an analytic correction to the analytic line-shape formula for constant excitation. The relevant integral is

$$P_1 = \int_0^\tau W_x(\tau,t)\left[(\pi/2)b_0\sin(\pi t/\tau) - b_0\right]\mathrm{d}t.$$

When the amplitude weight function for constant excitation is inserted, the integral can be evaluated as

$$P_1 = -\frac{{b_0}^2\Delta^2\tau}{p^3}\left[\frac{2\sin^2 p\tau}{p\tau} + \frac{\pi^2\sin 2p\tau}{4p^2\tau^2 - \pi^2}\right].$$

This correction is surprisingly good, illustrating the power of the method.

The corrected line shape is plotted in Fig. 3 together with the uncorrected line shape for constant excitation and the actual line shape for half-sine-wave excitation found by numerical integration of (3). Optimum power ($b\tau = \pi/2$) was chosen. The width of the approximate line shape is a little less than the width of the real line shape but much closer than the uncorrected line shape. However, where the real line shape goes to zero, the approximation becomes negative, an unphysical result.

A better approximation may be obtained by choosing τ' shorter than τ for the uncorrected line shape. The choice $\tau' = 0.74\tau$ matches the line widths of the uncorrected and actual line shapes. The correction then greatly improves the fit near the first null and matches the height of the first side lobe. For the range of detunings shown in Fig. 3, the difference between the corrected and actual line shapes is then no more than 1.5% of the peak height. For larger detunings, the weak-excitation approximation is better [3], [12].

B. Frequency Biases From Asymmetric Line Shapes

Phase and detuning perturbations introduce asymmetric corrections to the line shape, because the corresponding weight functions are antisymmetric in detuning. To find the resonance position in such cases, we consider slow square-wave modulation of the exciting frequency with amplitude ω_m. The resonance position is defined by that detuning $\delta\omega$ that makes the signals at the detunings

TABLE I. INHOMOGENEITY FUNCTIONS AND THEIR MEANS.

Name	$f(t)$	$f_{\rm m}$	$f_{\rm ms}$	f_x	f_x(small a)
Linear V	$\lvert 1-2t/\tau\rvert$	1/2	1/3	$1+\dfrac{(1+a^2/2)\cos a-1}{aD}$	3/8
Quadratic	$(1-2t/\tau)^2$	1/3	1/5	$(2\sin a+D)/3D-2/a^2$	1/5
Cosine	$\cos(2\pi t/\tau)$	0	1/2	$-a^2\sin a/(\pi^2-a^2)D$	$-3/\pi^2$
End steps	1, $0\le t\le\tau_1$ 0, $\tau_1\le t\le\tau-\tau_1$ 1, $\tau-\tau_1\le t\le\tau$	r	r	$\dfrac{[\sin a-\sin(a-ar)-ar\cos a]}{D}$	$r^2(3-r)/2$

In this table, $r=2\tau_1/\tau$ is the fraction of the excitation period occupied by the end steps and $D=\sin a-a\cos a$. When r is small, f_x for end steps has no term constant or linear in r, but is approximately $a^2r^2(\sin a-a\cos a/3)/2D$. This r dependence is a direct consequence of the weight function decreasing linearly to zero at the ends. The quantity f_x is generally less than one-half except when the line shape slope (proportional to D) is small.

$\omega_m+\delta\omega$ and $-\omega_m+\delta\omega$ equal. That is, we require the perturbed transition probabilities to match

$$P(-\omega_m+\delta\omega)+P_1(-\omega_m+\delta\omega)=P(\omega_m+\delta\omega)+P_1(\omega_m+\delta\omega).$$

Here we have emphasized the dependence of P on detuning and left its time dependence implicit. If we approximate P with a Taylor series

$$P(\omega_m+\delta\omega)\approx P(\omega_m)+\delta\omega\partial P(\omega_m)/\partial\omega, \quad (14)$$

the resonance position becomes

$$\delta\omega=-\frac{P_1(\omega_m)}{\partial P(\omega_m)/\partial\omega} \quad (15)$$

to first order in P_1. The denominator is the slope of the unperturbed line shape at a detuning corresponding to the modulation amplitude.

We could also approximate P in (14) by considering a perturbation that adds a constant shift $\delta\omega$ to ω. From the form of the unperturbed Hamiltonian and the definition of Δ, the perturbation would be $G_z=-(1/2)\delta\omega$. Then from (6) we would have the correction to P:

$$P_1=-\frac{1}{2}\delta\omega\int_0^\tau W_z(\tau,t)\,\mathrm{d}t. \quad (16)$$

Comparing (14) and (16), we see that, to first order in $\delta\omega$,

$$\partial P(\omega_m)/\partial\omega=-\frac{1}{2}\int_0^\tau W_z(\tau,t)\,\mathrm{d}t, \quad (17)$$

where W_z is also evaluated at the detuning ω_m. This relation can be used to provide an alternative expression for the denominator of the shift (15). For constant excitation, (17) can be verified analytically.

C. Inhomogeneity

A ubiquitous perturbation of frequency standards is the magnetic field seen by the atoms. This field often varies a little across the excitation region. Suppose the field amplitude can be described by a constant field H_0 plus a small addition H_1 $f(t)$, where H_1 denotes the change in amplitude and $f(t)$ contains all the time dependence and is of order unity. Then the bias due to the magnetic field can be described as a constant plus a small part linear in f, whether the bias is linear or quadratic in the total magnetic field.

We write the variable part of the bias as $\varepsilon\omega_0 f(t)$, where ε is very small [13]. The associated perturbation of the line shape is then given by

$$P_1=\int_0^\tau W_z(\tau,t)\frac{1}{2}\varepsilon\omega_0 f(t)\,\mathrm{d}t.$$

The associated frequency shift, given by (15), can then be expressed with the aid of (17) as $\delta\omega=\varepsilon\omega_0 f_x$, where the "excitation mean" f_x is given by the average of $f(t)$ with a normalized detuning weight function W_N defined by

$$W_N(\tau,t)=W_z(\tau,t)/\int_0^\tau W_z(\tau,t)\,\mathrm{d}t.$$

For constant excitation, W_N is given by [13]

$$W_N(\tau,t)=\frac{[\cos p_m(2t-\tau)-\cos p_m\tau]p_m}{\sin p_m\tau-p_m\tau\cos p_m\tau},$$

where $p_m^2=b^2+\omega_m^2/4$. Because W_z is symmetric about $\tau/2$, the excitation mean vanishes for any $f(t)$ antisymmetric about $\tau/2$.

In Table I [13], we list some sample symmetric functions $f(t)$, their mean (time average) $f_{\rm m}$, mean square $f_{\rm ms}$, their excitation mean f_x for constant excitation, and the value of f_x for small $a\equiv p_m\tau$. For half-sine-wave excitation, the excitation mean is even smaller, because the weight function is smaller where $f(t)$ is larger; compare Fig. 1(c).

TABLE II. TRANSITION AMPLITUDES AND WEIGHT FUNCTIONS FOR RAMSEY EXCITATION.

Region	$0 \le t \le \tau$	$\tau \le t \le \tau + T$	$\tau + T \le t \le \tau + T + \tau$
$\alpha(t)$	$\cos a'$	$\cos a \exp\left[i\Delta\left(t-\tau\right)\right]$	$\cos\,(a + a')\cos\Delta T$ $+ i\cos\,(a - a')\sin\Delta T$
$\beta(t)$	$-i\sin a'$	$-i\sin a \exp\left[-i\Delta\left(t-\tau\right)\right]$	$-\sin\,(a - a')\sin\Delta T$ $- i\sin\,(a + a')\cos\Delta T$
$W_x(\tau,t)$	$\sin 4a\cos^2\Delta T$	$\sin 4a\cos\Delta T\cos\Delta(2t - 2\tau - T)$	$\sin 4a\cos^2\Delta T$
$W_y(\tau,t)$	$\sin 2a\cos 2a'\sin 2\Delta T$	$-\sin 4a\cos\Delta T\sin\Delta(2t - 2\tau - T)$	$-\sin 2a\cos(2a - 2a')\sin 2\Delta T$
$W_z(\tau,t)$	$\sin 2a\sin 2a'\sin 2\Delta T$	$\sin^2 2a\sin 2\Delta T$	$\sin 2a\cos(2a - 2a')\sin 2\Delta T$

D. Sideband Pulling

In the rotating-wave approximation, a single sideband offset Ω from the excitation frequency ω with half Rabi amplitude b_1 and initial phase φ can be represented by

$$b_1 e^{\,i(\Omega t+\varphi)}.$$

The real part corresponds to amplitude modulation and does not cause a shift. The imaginary part corresponds to phase or frequency modulation and does cause a shift. From (6), the perturbation transition probability for the latter is

$$P_1 = \int_0^\tau W_y\left(\tau,t\right) b_1 \sin\left(\Omega t + \varphi\right) \mathrm{d}t.$$

If we add and subtract $(1/2)\Omega\tau$ to the argument of the sine, we can rewrite it as follows:

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

For excitations symmetric about $t = (1/2)\tau$, W_y is antisymmetric. The second term is symmetric; hence, its integral with W_y vanishes. The factor $\cos(\Omega\tau/2 + \varphi)$ in the first term is independent of t; hence, it may be removed from the integral, leaving

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

The cosine factor completely describes the dependence of P_1 and the corresponding shift on the initial phase. As discussed in [11], any thorough average over φ eliminates this first-order shift. The sideband pulling shift computed by Ramsey [14] (independent of initial phase) is second order in the sideband amplitude and cannot be obtained from our first-order weight functions.

For constant excitation, we can perform the integration analytically. The result is $P_1 = (2\Delta b/p^2)\sin p\tau X(\tau)$, where

$$X\left(\tau\right) = \frac{2b_1}{\left(\Omega^2 - 4p^2\right)}\left[\Omega\sin p\tau\cos\frac{1}{2}\Omega\tau - 2p\cos p\tau\sin\frac{1}{2}\Omega\tau\right] \times \cos\left(\frac{1}{2}\Omega\tau + \varphi\right).$$

When we insert this P_1 into (15), we obtain the Rabi sideband pulling shift

$$\delta\omega = \frac{2p^2 X\left(\tau\right)}{b\left(\sin p\tau - p\tau\cos p\tau\right)}.$$

This is the same shift given in (11) and (12) of [11]. By using the weight function, we have bypassed much of the derivation given in [11].

IV. PERTURBATIONS IN RAMSEY EXCITATION

Ramsey excitation consists of 2 short, usually identical, periods of excitation separated by a relatively long "drift" interval T free of excitation. To use weight functions with Ramsey excitation, we must understand that the probability amplitudes defined by (7)–(9) now refer to the complete cycle of excitation. We must therefore express them in 3 consecutive time intervals spanning both excitations. For simplicity, we shall assume that we can ignore detuning during excitation. We introduce the abbreviation $a' = \int_0^t b\left(t'\right)\mathrm{d}t'$ for the integrated excitation. We write a for a' evaluated at $t = \tau$. For constant excitation, $a' = bt$ and $a = b\tau$. For half-sine-wave excitation, $a' = b_0\tau\sin^2(\pi t/2\tau)$ and $a = b_0\tau$. Table II shows α and β in the 3 time intervals using these abbreviations. We then used (7)–(9) to construct the 3 Ramsey weight functions in the 3 time intervals, as also shown in Table II. The symmetries of these weight functions are the same as given earlier. But note that the time symmetry is now about the midpoint of the drift interval (time of apogee for fountains).

Figs. 4(a)–(c) show the shape of the 3 weight functions as a function of time for $T = 4\tau$ and $2a = 0.79\pi/2$ (2 dB below optimum excitation). Because of the factor $\cos 2a$, all of W_x and the central part of W_y vanish when the excitation is exactly optimum. The difference between constant and half-sine-wave excitation is only in the excitation regions and primarily affects the slopes of the weight functions at either end of the excitation regions.

From the final value of $\beta(t)$ we find the unperturbed transition probability,

$$P = \frac{1}{2}\sin^2 2a\left(1 + \cos 2\Delta T\right),$$

and its derivative with respect to detuning,

$$\partial P/\partial\omega = -\frac{1}{2}T\sin^2 2a\sin 2\Delta T. \tag{18}$$

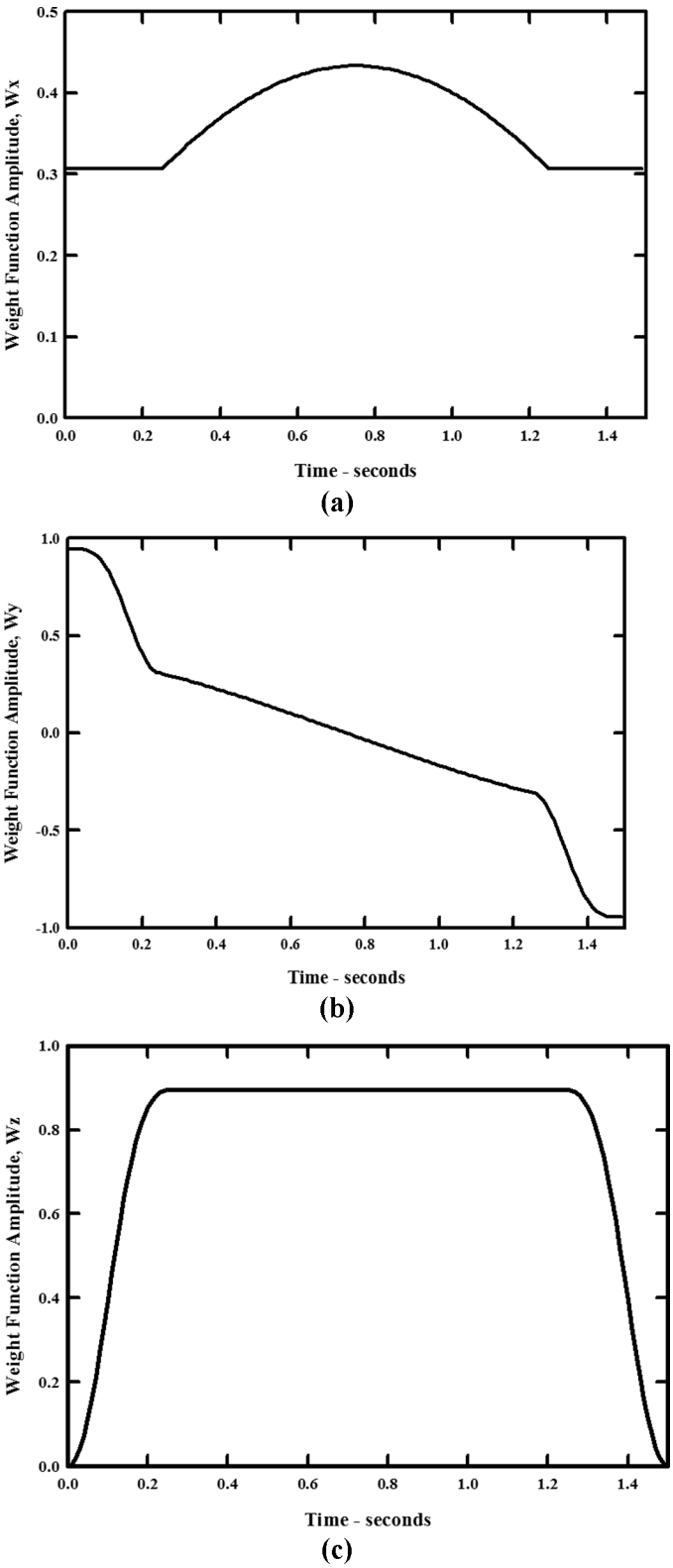

Fig. 4. Weight functions for half-sine-wave Ramsey excitation numerically evaluated at 2 dB below optimum power and small (one half fringe width) detuning. The artificial ratio $T/\tau = 4$ was chosen to bring out the time dependence during excitation. (a) Amplitude weight function, (b) phase weight function, and (c) detuning weight function.

For slow frequency modulation, we can use (15) and (18) evaluated at the detuning $2\Delta = \omega_m$ to convert a perturbation transition probability into a shift of a Ramsey fringe. We have assumed only that the shift is small compared with the fringe spacing.

A. Asymmetry of Excitation in Fountains

In cesium fountains, the atoms are slowing as they go up through the first excitation region and accelerating as they come back down. Thus, the time intervals spent by the atoms in the first and second halves of the excitation cavity are not equal. If the excitation amplitude is not constant in space, the atoms see an excitation amplitude asymmetric in time during each pass through the cavity, even though the overall Ramsey excitation may be symmetric in time. From Table II, we see that the amplitude weight function is constant in the excitation regions. Hence, the first-order perturbation caused by any asymmetry of the excitation amplitude averages to zero. There is no effect on the Ramsey line shape. This remains true even if the 2 excitations have unequal amplitudes, provided their average amplitude is used. Unequal excitation amplitudes may occur when an atom's average trajectory does not pass at the same distance from the cavity axis on both transversals.

B. Inhomogeneity

Consider first that the atomic resonance ω_0 is changing, as it might in an inhomogeneous magnetic field. For changes occurring during the drift time, Table II shows that W_z is constant. Hence, the unweighted time average of ω_0 will appear; compare [3, eq. (49)]. However, changes in ω_0 during excitation are weighted toward the end of the first excitation and the beginning of the second excitation (toward the top of the excitation cavity in fountains). Inhomogeneity at either end of the total Ramsey excitation is underweighted.

As an example of a change in resonance, consider that light scattered from atom preparation is not cut off before some atoms enter the excitation region. That is, the resonance frequency ω_0 is perturbed by a shift $\delta\omega_S$ that is present for only a short period t_S at the beginning of the first excitation. The perturbation can then be described by $G_z = 1/2\delta\omega_S$ for $0 \le t \le t_S$ and 0 for larger t values. From (6) and Table II, the associated perturbation probability becomes

$$P_1 = \frac{1}{2}\sin 2a \sin \omega_m T \int_0^{t_S} \sin 2a' \mathrm{d}t\, \delta\omega_S.$$

For t_S much smaller than τ, $2a'$ will be small enough that $\sin 2a'$ can be replaced by $2a'$. The Ramsey shift associated with this perturbation then becomes

$$\delta\omega_R = -\frac{\delta\omega_S}{2T \sin 2a} \int_0^{t_S} 2a' \mathrm{d}t.$$

For constant excitation, $2a' = 2bt$, and the integral becomes $bt_S{}^2$. For half-sine-wave excitation, $2a' \approx (1/2)\, b_0 t^2/\tau$, and the integral becomes $(\pi^2/6) b_0 t_S{}^3/\tau$. The shift for half-sine-wave excitation is smaller than the shift for constant excitation by the factor t_S/τ, due to the less abrupt turn-on of the excitation. More gradual turn-offs than the sharp cutoff assumed above reduce the coefficient in the evaluated integrals. Alternatively, we can say that gradual turn-offs allow larger values of t_S.

The next 4 perturbations are all treated using the *same* phase weight function W_y. However, the range of integration varies with the time-dependence of each perturbation.

C. End-to-End Phase Shift

Assume that the phase of the excitation in the second excitation region differs from that in the first by $\delta\theta$, but that the phases are otherwise constant. We can describe this by considering $\delta\theta$ to be a phase perturbation in only the second excitation region. For a small phase change, the phase perturbation is $G_y = b(t)\delta\theta$. The perturbation probability becomes

$$P_1 = \int_{\tau+T}^{\tau+T+\tau} W_y(\tau,t)\, b(t)\, \delta\theta \mathrm{d}t,$$

where the integration is carried only over the second excitation region. From Table II, the only part of W_y in the second region that depends on t is a'. Because b is the derivative of a', the integral can be performed, yielding

$$P_1 = -\frac{1}{2}\delta\theta \sin^2 2a \sin 2\Delta T.$$

From (15) and (18), we then find the Ramsey resonance shift $-\delta\theta/T$, independent of excitation or modulation amplitude. This reproduction of a familiar result illustrates the wide applicability of the weight function analysis.

D. Excitation Leakage Into the Drift Region

Biases due to leakage of excitation fields out of the nominal excitation region have been discussed in [15]. From the detuning symmetry of (3) and the weight functions, we know that only that part of any excitation field leakage out of phase with the primary excitation causes a shift. For leakage during the drift time, we also see that the leakage amplitude must be partly antisymmetric in time to cause a shift, because the phase weight function is antisymmetric. As an artificial example having a nonzero shift, consider a constant weak excitation of amplitude b_L for a period t_L less than T beginning immediately after the first excitation. From the phase weight function we find the perturbation probability is

$$P_1 = \int_{\tau}^{\tau+t_L} W_y(\tau,t)\, b_L \mathrm{d}t = (b_L/\Delta)\sin 2a \cos 2a \cos \Delta t_L \times \left[\cos\Delta(T - 2t_L) - \cos\Delta T\right].$$

This result agrees with (14) and (15) in [15]. For t_L equal to half of T, it reduces to half the error signal in (16) of [15].

For leakage before or after Ramsey excitation, the definition of our weight functions must be extended to include the leakage region.

E. Distributed Cavity Phase

Biases due to distributed cavity phase variations in cesium fountains have been discussed in [16]. We illustrate here how the same results can be obtained by using the phase weight function shown in Table II. Let $b_1'(t)$ and $b_2'(t)$ represent the cavity field amplitudes in phase quadrature with the primary excitation field during the first and second excitations, respectively. The perturbation transition probability is then

$$P_1 = \int_0^{\tau} W_y(\tau + T + \tau, t) b_1'(t)\mathrm{d}t + \int_{\tau+T}^{\tau+T+\tau} W_y(\tau + T + \tau, t) b_2'(t - \tau - T)\mathrm{d}t.$$

Inserting the phase weight function from Table II we can write this

$$P_1 = \sin 2a \sin 2\Delta T \times \int_0^{\tau} [\cos 2a'\ b_1'(t) - \cos(2a - 2a') b_2'(t)]\mathrm{d}t, \quad (19)$$

where the time argument in the second term has been readjusted to the same range as for the first term. If we substitute the definitions of ε and η from [16, eq. (9)] into [16, eq. (14)] and apply trigonometric identities, we can show that [16, eq. (14)] is equivalent to (19). For the example given in [16], b_1 is zero and b_2 is proportional to $(t/\tau - 1/2)^2$. For half-sine-wave excitation $2a - 2a' = b\tau[1 + \cos(\pi t/\tau)]$. Expanding the cosine of this argument then leads to the same results given in (17) of [16].

F. Sideband Pulling

As in the Rabi case, we can find the perturbation effect of a sideband by integrating the associated phase perturbation $G_y = b_1 \sin(\Omega t + \varphi)$ with the Ramsey phase weight function. The integration extends only over the 2 excitation regions. But note that in the second region, φ will be replaced by $\varphi + \Omega\tau + \Omega T$. This change accounts for the sideband's phase advance at the later time.

For symmetric excitation about the mid-time $t = T/2 + \tau$, W_y is antisymmetric. We can then factor out the initial phase dependence just as we did in the Rabi case. We find

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

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

$$P_1 = \frac{2b_1 Y(T,\tau)}{\Omega^2 - 4b^2}\sin 2a\,\sin 2\Delta T\cos\left(\frac{1}{2}\Omega T + \Omega\tau + \varphi\right),$$

where

$$Y(T,\tau) = \Omega\cos\left(\frac{1}{2}\Omega T + \Omega\tau\right) - \Omega\cos 2a\cos\left(\frac{1}{2}\Omega T\right) + 2b\sin 2a\sin\left(\frac{1}{2}\Omega T\right).$$

The shift due to the sideband perturbation is then

$$\delta\omega = \frac{4b_1}{T\left(\Omega^2 - 4b^2\right)\sin 2a}Y(T,\tau)\cos\left(\frac{1}{2}\Omega T + \Omega\tau + \varphi\right),$$

in agreement with (15) in [11]. However, the derivation here is much shorter.

Our first-order weight functions do not predict the much smaller second-order Ramsey sideband pulling shift, which is independent of the initial phase [17].

V. Summary

We have expressed the first-order effect of a perturbation on the 2-level transition line shape as a time integral over the perturbation with a weight function independent of the perturbation. We have introduced 3 different weight functions for the 3 different types of perturbation. A weight function needs to be calculated only once to be used for any perturbation of its type. We have thereby unified the derivation of shifts due to several disparate perturbations. We have presented several examples of the use of these weight functions to predict line-shape changes and frequency biases.

Appendix
Relation of the Detuning Weight Function to the "Sensitivity Function"

In developing the theory of the "Dick effect" in atomic frequency standards, the so-called sensitivity function was introduced [5], [7], [18]. It has been defined as the response of the atomic system to a small step in the phase of the excitation. We carry out this definition here to show the equivalence of the sensitivity function to the detuning weight function W_z.

We consider a small phase step $\delta\theta$ occurring at time t and continuing for the remainder of the excitation. The corresponding phase perturbation is $b\delta\theta$ times a unit step function starting at time t. The corresponding small change in transition probability is this perturbation averaged from time t onward with the phase weight function:

$$\delta P(t) = \int_t^\tau W_y(\tau,t')b(t')\delta\theta\,\mathrm{d}t'.$$

From the last of the differential equations (12), we can rewrite this as

$$\delta P(t) = \frac{1}{2}\delta\theta\int_t^\tau \frac{\partial W_z(\tau,t')}{\partial t'}\,\mathrm{d}t'.$$

Because W_z vanishes at the upper limit, we are left with

$$\delta P(t) = -\frac{1}{2}W_z(\tau,t)\delta\theta.$$

From [18], the sensitivity function $g(t)$ is defined as twice the change in the transition probability due to a phase step in the limit of a small phase step. In our notation, this becomes

$$g(t) \equiv 2\delta P(t)/\delta\theta = -W_z(\tau,t).$$

This result could also have been obtained directly from (13) by recognizing that the derivative of a step function is the Dirac delta function.

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