Velocity Distributions Calculated from the Fourier Transforms of Ramsey Lineshapes

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Abstract—A computerized method for finding velocity distributions from the Fourier transforms of Ramsey lineshapes has been developed. Experimental and numerical tests of the method show that it works very well for broad distributions and lineshapes where the drift time is much longer than the excitation time. The method is routinely used to find velocity distributions for the primary frequency standard NIST-7. The second-order Doppler shift is calculated from these distributions with an uncertainty of a few tenths of 1 percent.

Index Terms—Fourier transform, frequency standard, NIST-7, Ramsey lineshape, second-order Doppler shift, transit time, velocity distribution.

I. INTRODUCTION

WHEN AN atomic resonance is observed using the method of separated oscillating fields [1], the resulting interference resonance curve is called a Ramsey lineshape or Ramsey fringe. An early paper by Daams [2] first suggested that information about the atomic velocity distribution is contained in the Fourier transform of such a Ramsey lineshape. The idea was further developed by the author with the inclusion of data taken at different excitation powers [3]. Considerable experience in using the method has now been obtained using both theoretical and experimental data.

A similar method was developed independently by Jarvis [4]. He also starts with Ramsey lineshapes at several powers, but uses a lineshape-specific transform, rather than a Fourier transform. This introduced some ambiguities. Other methods for obtaining velocity distributions are based on pulsed microwave excitation [5], [6] or power dependence of the signal [7]. These methods use experimental data of less accuracy. Hence they cannot obtain the precision required for NIST-7. With optically-pumped standards a direct time-of-flight method can be used [8]. It agrees well with the present method, but requires correction for the frequency response of the detector.

We describe below the basic theory of our method and firstorder corrections. The effect of the Rabi pedestal is discussed briefly. We then describe results of several tests made with the method. Finally we describe how the second-order Doppler correction is obtained from the transit-time distribution.

Manuscript received June 20, 1996; revised October 1, 1996.

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Publisher Item Identifier S 0018-9456(97)02131-1.

II. BASICS OF THE METHOD

A. The Fourier Transform Relation

We consider an atomic beam spectrometer with a horizontal thermal beam traversing two identical excitation regions. When the drift region length L is much longer than the excitation region length ℓ , the Ramsey lineshape can be represented approximately by the expression [1]

$$P(\lambda) = \int_0^\infty \rho(T) \sin^2(2b\tau) \cos^2(\frac{1}{2}\lambda T) \, dT. \tag{1}$$

Here $\tau = \ell/v$ and T = L/v are the transit times for an atom of velocity v across the excitation and drift regions respectively, 2b is the Rabi frequency (proportional to the microwave field strength), and $\lambda = \omega - \omega_0$ is the detuning of the exciting frequency ω from the atomic resonance frequency ω_0 . The $\sin^2(2b\tau)$ factor represents the Rabi excitation probability for the two excitation regions without a drift region. The $\cos^2(\frac{1}{2}\lambda T)$ factor introduces the interference developed during the drift time between excitations. The atomic velocity average is represented by the integral over the distribution $\rho(T)$ of transit times T. Two sample Ramsey lineshapes are shown in Fig. 1.

If we use the half-angle formula to expand the interference factor in (1), we obtain

$$P(\lambda) = \frac{1}{2}R(0) + \frac{1}{2}R(\lambda), \tag{2}$$

$$R(\lambda) = \int_0^\infty \rho(T) \sin^2 aT \cos \lambda T \, dT \tag{3}$$

where $R(\lambda)$ is the Ramsey fringe pattern and R(0) is the underlying Rabi pedestal. The coefficient *a* is an abbreviation for $2b\ell/L$. For a distribution $\rho(T)$ of finite width, $R(\lambda)$ approaches 0 for large λ . Equation (3) shows that the Ramsey fringe pattern is just the Fourier cosine transform of the transit-time distribution times the transition probability [3]. By inverting the transform we can recover the integrand. Fig. 2 shows the inverted transforms of the lineshapes shown in Fig. 1.

To recover the transit-time distribution alone, we must divide the inverse Fourier transform of $R(\lambda)$ by the transition probability. There are two difficulties in doing so. First, the transition probability is very small for certain transit times making the result of division inaccurate. Second, the transition probability is not well known because the Rabi frequency 2bis not well known. It can be determined approximately from



Fig. 1. Experimental Ramsey lineshapes for NIST-7. (a) 1.85 dB above optimum power. (b) 3.13 dB below optimum power.



Fig. 2. Fourier transforms of the Ramsey lineshapes shown in Fig. 1. (a) 1.85 dB above optimum power. (b) 3.13 dB below optimum power.

 $T_m = \pi/a$, the value of T that makes the transition probability vanish. But, as Fig. 2(a) shows, T_m is not well determined either. These difficulties will be resolved in the next section.

B. Use of Multiple Ramsey Lineshapes

The transform of a single Ramsey pattern gives an incomplete picture of $\rho(T)$ since the $\sin^2 aT$ factor suppresses information about $\rho(T)$ near $T_m, 2T_m, \cdots$ To complete the picture we use Ramsey fringe data at different microwave excitation powers (different *a* values). In these data, information about different regions of $\rho(T)$ will be suppressed. We adopt the criterion that data will not be used in regions where $\sin^2 aT$ is less than a cutoff value W_c , typically 0.25. Fig. 3 illustrates how the powers used for taking Ramsey lineshape data with NIST-7 then cover the range of *T*. The solid bars show the regions in *T* where the Ramsey fringe at that power provides information about the velocity distribution. The gaps correspond to regions where the data is not used because the transition probability is small. There is always a gap at the smallest values of *T*. But we expect $\rho(T)$ to vanish there, since small T values correspond to high velocities which are cut off by a Maxwell distribution in the beam source.

For most regions of T we now have data from transforms at several power levels. We combine the data as follows. Let the index j denote the power level. From each measured Ramsey fringe $R_j(\lambda)$, we obtain a Fourier transform $F_j(T)$. We define trial distributions by

$$\rho_j(T) = F_j(T) / \sin^2 a_j T. \tag{4}$$

We then form a weighted average of the trial distributions:

$$\overline{\rho}(T) = \sum_{j} \rho_j(T) W_j(T) / \sum_{j} W_j(T).$$
(5)

For a weighting function we choose $W_j(T) = \sin^4 a_j T$, the square of the Rabi transition probability. When the transition probability is less than our cutoff W_c , we set the weighting function to zero. This weighting function softens the cutoff edge.

In this combination process it is important to retain the relative amplitudes of the Ramsey fringes and their transforms



Fig. 3. Regions of transit time T for which the transition probability is greater than 0.25. The corresponding power levels relative to optimum are shown on the left.

at the various powers. Useful information is thereby preserved. Absolute amplitudes are irrelevant since the final distribution $\overline{\rho}(T)$ will be normalized so that its integral over T is 1.

C. The Quality-of-Fit Parameter

To get a measure of how closely the trial distributions agree with each other, we introduce the quality-of-fit parameter

$$E(a) = \int_0^\infty D(T) \, dT \tag{6}$$

where

$$D(T) = \sum_{j} [\rho_j(T) - \overline{\rho}(T)]^2 W_j(T)$$
(7)

is the mean square deviation of ρ_j from $\overline{\rho}$ at each T value, weighted by $W_j(T)$. Our choice of weighting function makes E equivalent to the sum of the mean square errors between the input lineshapes $R_j(\lambda)$ and lineshapes computed from the fitted distribution $\overline{\rho}(T)$.

The quality-of-fit parameter can be used to determine the power scale. If the ratio of microwave powers can be accurately determined, then the ratios of the a_j are known. When the quality-of-fit parameter E is plotted against one of the a values, we obtain a curve like that shown by the broken line in Fig. 4. The minimum is three orders of magnitude deep and defines a within 0.5%.

The depth of the minimum in the quality-of-fit parameter reflects the noise on the lineshape data. It can be used as a rough measure of the quality of the lineshape data, and hence the accuracy of the distribution obtained.

III. CORRECTIONS TO THE THEORY

A. First Order in ℓ/L

The distributions obtained from the basic theory are systematically shifted in T by an increment of order τ . To correct for this shift, we replace (3) by

$$R(\lambda) = \int_0^\infty \rho(T) \sin^2 aT \cos \lambda (T + h\tau) \, dT. \qquad (8)$$



Fig. 4. Variation of the quality-of-fit parameter E with the a value for optimum power. The broken curve is without the ℓ/L correction and the solid curve is with the correction.

where *h* is a dimensionless function. $\lambda h\tau$ is twice the firstorder phase correction to the quantum-mechanical amplitude that no transition occurs in one excitation region. This phase correction also appears in the calculation of the frequency shift of the Ramsey fringe when the atomic resonance frequency in the excitation regions is different from the resonance frequency in the drift region [9]. Correspondingly we replace (4) by

$$\rho_j(T) = \frac{F_j(T+h\tau)}{\sin^2 aT} [1 - (\ell/L)(h+b\tau h')]^{-1} \qquad (9)$$

where h' is the derivative of h.

The function $h(b\tau)$ depends on the microwave field profile seen by atoms as they traverse the excitation region. For a rectangular profile found in most standards using transverse magnetic fields we have

$$h(b\tau) = \tan(b\tau)/b\tau.$$
 (10)



Fig. 5. Transit time distribution for NIST-7 obtained from data including that shown in Figs. 1 and 2.

For a half-sine-wave profile found in most standards using longitudinal C-fields, we have

$$h(b\tau) = J_0(b\tau) \sec(b\tau) \tag{11}$$

where J_0 is the Bessel function of zero order. For either profile h is close to 1 for small values of $b\tau$. The singularity at $b\tau = \pi/2$ is not real; it occurs where the transition probability has a zero.

When (9) is used in place of (4), the average distribution is no longer shifted in T. The quality-of-fit parameter assumes a shape like that shown by the solid line in Fig. 4. The minimum is deeper, more sharply defined, and shifted to the correct value. The corresponding transit-time distribution $\overline{\rho}(T)$ is shown in Fig. 5. This distribution is typical of those for NIST-7. It has fewer low velocity atoms than a thermal distribution weighted by 1/v for detection by a cycling optical transition.

B. Effect of the Rabi Pedestal

The Rabi pedestal is not actually constant across the Ramsey fringe, as (2) implies, but curves up or down, depending on the excitation power. Since the Ramsey fringe data extend only to a cutoff frequency ν_c , the pedestal curve is broken there. Beyond ν_c the data are assumed constant. The Fourier transform of the broken pedestal curve is a damped oscillation like that shown in Fig. 2 at small *T*. The oscillation frequency is ν_c and the damping is proportional to $(\nu_c T)^{-2}$. If we choose ν_c large enough, we push the transform of the pedestal to small enough *T* that the residual oscillation underlying $\rho(T)$ does not seriously degrade it. The Fourier transforms of computergenerated Ramsey fringes without the Rabi pedestal show a similar, but smaller, residual oscillation at small *T*.

IV. TESTS OF THE METHOD

A. Numerical Tests

The numerical method has been tested by starting with known transit-time distributions. Ramsey lineshape data were generated at four powers from theoretical formulas for the complete lineshape. The lineshapes were then transformed and transit-time distributions recovered. The recovered distributions agree very well with the originals. The agreement is best for broad distributions of finite range, such as we actually observe in NIST-7.

Errors in relative power were intentionally introduced. Changes of 0.1 dB in one of the input powers caused the quality-of-fit parameter to increase by factors between 2 and 10, but the mean and root-mean-square transit times changed less than 0.1%. The distributions also were not significantly affected when the cutoff W_c was varied from 0.18 to 0.45.

A special test was made starting with an experimental distribution. Ramsey lineshapes were computed theoretically, transformed, and a reconstituted distribution obtained. This procedure was then repeated two more times using the successive reconstituted distributions as input to the next stage. Comparing the final thrice-reconstituted distribution with the original we found the major difference to be a small decrease near the extremes of the distribution. Mean transit times agreed to 0.2%.

Additional tests were made adding computer generated noise to the lineshape data. The quality-of-fit parameter was thus found to be proportional to the square of the amplitude of the added noise.

B. Experimental Tests

The method has now been applied to lineshape data from NIST-7 for over two years. Data are taken from 0 to 512 Hz detuning on one side of the line at 4 Hz intervals. The powers

are approximately +2.5, 0.0, -2.5, and -5.0 dB where 0 dB is optimum power: that power maximizing the dc signal at zero detuning. The Fourier cosine transform is performed on 512 points, corresponding to 1024 points if both sides of the lineshape were used. The fitted distribution typically contains about 100 points extending from T = 2 to T = 28 ms.

The transit-time distributions thus obtained from experimental lineshape data have been remarkably consistent. No significant change occurs when powers or data spacing are varied. Changes in oven temperature of 5 °C can be easily seen when the corresponding distributions are compared. Differences of 1% to 3% between the distributions for the west-to-east beam and the east-to-west beam are routinely seen and accounted for in processing frequency data. The distributions also agree well with those measured by a pulsed optical pumping technique [8]. The distributions have been used to compute the shape of the Rabi pedestal at various powers. Good agreement with experiment was found.

To test reproducibility, sixteen sets of Ramsey fringe data for NIST-7 were taken consecutively in an hour's time with no change in operating conditions. The transit-time distributions obtained differed by less than 1%. The mean transit times had a scatter of only 0.1%.

V. COMPUTATION OF THE SECOND-ORDER DOPPLER SHIFT

The second-order Doppler shift is computed from the ratio of two integrals over the transit-time distribution:

$$\Delta \omega_D / \omega_0 = (L^2 / 2c^2) (M_0 / M_2) \tag{12}$$

where c is the velocity of light

$$M_0 = \int_0^\infty \overline{\rho}(T) \sin^2 aT \sin \omega_m T \, dT \tag{13}$$

and M_2 is the same integral with an additonal factor T^2 in the integrand. The sin $\omega_m T$ factor, where ω_m is the modulation amplitude, takes into account the slow squarewave modulation used for measuring the resonance frequency. Because the shift is a ratio of two integrals, any errors in the transit-time distribution partially compensate making the shift less sensitive to $\rho(T)$. The sixteen experimental distributions gave shifts having a scatter of less than 0.2%, or 10^{-15} of the cesium frequency.

VI. CONCLUSIONS

The Fourier transform method of obtaining velocity distributions from Ramsey lineshapes is capable of good accuracy (less than 1%) for broad, smooth distributions and small ℓ/L ratios. Our experience with the method and specific tests give us confidence that average quantities like the mean transit time and the second-order Doppler shift can be computed from these transit-time distributions with an uncertainty of only a few tenths of 1 percent.

REFERENCES

- N. F. Ramsey, *Molecular Beams*. Oxford, U.K.: Oxford Univ. Press, 1956, sect. V.4.2, pp. 127–131.
 H. Daams, "Corrections for second-order Doppler shift and cavity
- [2] H. Daams, "Corrections for second-order Doppler shift and cavity phase error in Cesium Atomic beam frequency standards," *IEEE Trans. Instrum. Meas.*, vol. IM-23, pp. 509–514, Dec. 1974.
 [3] J. H. Shirley, "Velocity distributions from the Fourier transforms of
- [3] J. H. Shirley, "Velocity distributions from the Fourier transforms of Ramsey line shapes," *Proc. 43rd Symposium on Frequency Control*, June 1989, pp. 162–165.
- [4] S. Jarvis, "Determination of velocity distributions in molecular beam frequency standards from measured resonance curves," *Metrologia*, vol. 10, pp. 87–98, 1974.
- [5] A. De Marchi, G. D. Rovera, and A. Premoli, "Pulling by neighboring transitions and its effects on the performance of Cesium-beam frequency standards," *Metrologia*, vol. 20, pp. 37–47, 1984.
- [6] H. Hellwig, S. Jarvis, D. Halford, and H. E. Bell, "Evaluation and operation of atomic beam tube frequency standards using time domain velocity selection modulation," *Metrologia*, vol. 9, pp. 107–112, 1973.
- [7] J.-S. Boulanger, "A new method for the determination of velocity distributions in Cesium beam clocks," *Metrologia*, vol. 23, pp. 37–44, 1986.
- [8] W. D. Lee, J. H. Shirley, and R. E. Drullinger, "Determining the velocity distribution of atomic beams by gated optical pumping," *Proc. 48th Symposium on Frequency Control*, 1994, pp. 658–661.
 [9] J. Vanier and C. Audoin, *The Quantum Physics of Atomic Frequency*
- [9] J. Vanier and C. Audoin, *The Quantum Physics of Atomic Frequency Standards*, Bristol, U.K.: Adam Hilger, 1989, sect. 5.6.3, pp. 801–803, and references therein.



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