

# Minimizing the optical frequency shifts of a rubidium discriminator

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Questions concerning the long-term stability of a rubidium frequency discriminator are analyzed. Numerical simulation has been used to study the effect of the optical-pumping regime and the isotopic-filtering regime on the frequency shifts of the reference 0-0 transition in the hyperfine structure of the  $^{87}\text{Rb}$  ground state and on the quality parameter of the 0-0 resonance. Recommendations are offered on the basis of a joint optimization of the regimes of the pump source, the isotopic filter, and the working cell. It is shown that there are no pumping regimes which would make the frequency of the 0-0 transition independent of the entire set of parameters of the discriminator. The only radical step which can be taken to improve the long-term stability is to reduce the intensity of the pump light to the minimum level which provides the required value of the quality parameter. Results of an experimental test of the relations found here are reported. Practical recommendations are offered regarding the choice of discriminator regimes.

1. In our previous papers<sup>1-4</sup> we have re-examined the conventional approach to choosing the intensity of the optical pump in a rubidium frequency standard. It has been shown that consideration of the actual sources of noise in the detection of the double-resonance signal – the shot noise in the photocurrent and the amplitude-phase fluctuations of the microwave field – leads to the conclusion that the optimum intensity of the pump light is sharply lower (by a factor of tens) than the intensity which is used in practice. At this lower pump intensity, the resolution of an atomic frequency discriminator with the actual sources of noise is maximized, and – a particularly important point – the parametric instabilities of

the resonant frequency associated with the pump light (optical frequency shifts) are lowered by a factor of tens. We know that in addition to the direct dependence of the resonant frequency on the pump light intensity  $I$  the optical shifts are manifested as cross-effect such as a dependence of the temperature coefficient of the resonant frequency on the intensity of the pump light, frequency shifts related to the microwave field power and the modulation parameters, a dependence of the frequency on the regimes of the isotopic filter, etc. All of these shifts are proportional to the intensity of the pump light, so lowering this intensity is desirable from all standpoints.

The primary method which has been used

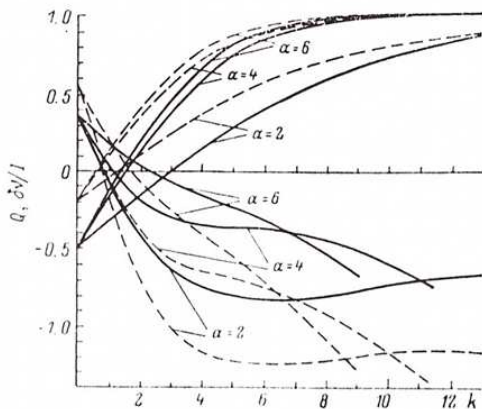


FIG. 1. Solid lines)  $\kappa = 0$ ; dashed lines)  $\kappa = 2$  (self-inversion of the pump).

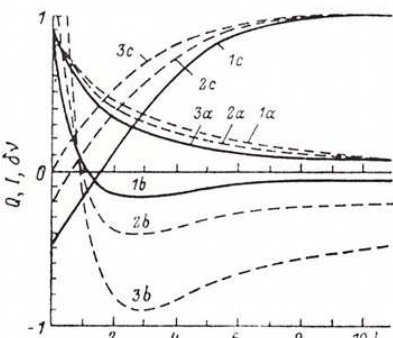


FIG. 2. 1)  $\kappa = 0$ ; 2)  $\kappa = 2$ ; 3)  $\kappa = 4$ . a - The pump intensity  $l$ ; b - the optical shift  $\delta\nu$ ; c - the pumping efficiency  $Q$ .

to combat optical shifts has been to carefully match and stabilize the regimes of the various elements of the discriminator (the light source, the isotopic filter, and the resonant cell), in which the optical and temperature shifts are minimized simultaneously. Reducing the intensity of the pump light relaxes the requirements on the stability of these regimes, eliminates the cross-dependence of the frequency, and thus reduces the long-term frequency drift. In addition, lowering the intensity of the pump light opens up some additional possibilities for organizing the pumping and the operating regimes of the various elements of the discriminator in searches for optimum combinations of these factors. We have in mind here a wide variation of the spectral composition of the pump light. The requirement of a substantial pump power level, which has prevailed in the past, has ruled out the use of radiation in one of the lines  $D_1$ ,  $D_2$  (because to single out one of these lines is to suffer an optical loss by a factor of three to ten), has ruled out the use of a dense isotopic filter, and has ruled out the use of the spectral lamp in any regime other than that close to maximum brightness.

Under the new conditions it has become an urgent matter to analyze the effect of the spectral characteristics of the pump light on the magnitude of the optical shifts. In the present paper we are reporting the results of a theoretical and experimental study of the optical shifts of the rubidium 0-0 resonance as functions of the regimes of the lamp and the isotopic filter, separately for the two resonant lines of Rb. This study makes it possible to formulate some additional recommendations

aimed at increasing the long-term frequency stability of a rubidium standard.

2. The general scheme for calculating the optical shifts of the energy levels of an atom is well known.<sup>5</sup> However, using this scheme in practice to calculate the optical shift  $\delta\nu$  of the line of a double rf-optical resonance is extremely tedious and it runs into difficulties which stem from the uncertainty regarding the spectral lineshape of the pump. We have used a simplified calculation scheme in which the lineshape is specified by analytic models, and the volume to be pumped is assumed to be optically thin. The effect of a nonzero optical thickness can be estimated easily by introducing a corresponding transformation in the pump spectrum. Under these simplifying assumptions we have carried out numerical calculations of the optical shift as a function of the optical density of the isotopic filter. We specified a grid of buffer-gas densities in the filter and varied the spectral lineshape of the pump. The results of some model calculations have been used to plan actual measurements.

Let us review the optical layout of a rubidium standard. After one of the lines  $D_1$ ,  $D_2$  is selected from the light from an  $^{87}\text{Rb}$  lamp (or without this preliminary conversion to a monochromatic spectrum), the light passes through an isotopic filter which contains  $^{85}\text{Rb}$  vapor with a buffer gas. The light then performs an optical pumping in the working volume, with  $^{87}\text{Rb}$  vapor, with a small amount of a mixture of buffer gases.

In the calculations, the spectral lineshapes of the absorption of the filter and of the working volume are described as a sum of hyperfine components with a Voigt shape. The Voigt parameter  $a = \Delta\nu_c/2\Delta$  ( $\Delta = \Delta\nu_D/2\sqrt{\ln 2}$  is the reduced Doppler linewidth, and  $\Delta\nu_c$  is the homogeneous width) is assumed to be 0.1, with  $\Delta = 330$  MHz (330 K). As the buffer gas in the filter we select nitrogen, which quenches the resonant luminescence of rubidium. We assume that the broadening of the line  $D_1$  by nitrogen is 18 MHz/torr, and the shift is  $-7$  MHz/torr; for the line  $D_2$  we adopt 18.9 and  $-8.2$  MHz/torr, respectively. We assume a reduced width of 360 MHz. We vary the parameter  $a$  for the filter over a wide range. The models of the spectral lineshapes of the pump are based on the same layout, in which the parameters  $a$  and  $\Delta$  are assumed to be 0.2 and 400 MHz.

Figure 1 illustrates the results with a calculated family of curves of the relative shift  $\delta\nu/l$  of the frequency of the 0-0 resonance caused by the line  $D_2$ , plotted as a function of the optical density of the  $^{85}\text{Rb}$  vapor in the filter. Specifically, the quantity plotted along the abscissa is the density at the maximum of the most intense component of the hyperfine spectrum. The dashed lines here show a corresponding family of curves calculated under the condition that the emission from the course has undergone a self-absorption with an absorber density  $\kappa$  having a value of 2 at the maximum. The dashed lines give an idea of the nature of the changes caused in the optical shift as the lineshape varies as a result of self-inversion in the lamp or self-absorption in the working volume.<sup>1)</sup> Also shown here are curves of the pumping efficiency

$$Q = (W_1 - W_2)/(W_1 + W_2), \quad (1)$$

where  $W_1$  and  $W_2$  are the rates of excitation of  $^{87}\text{Rb}$  atoms from the  $F = 1$  and  $F = 2$  hyperfine

sublevels, respectively, as a function of the filter density  $k$ .

Figure 2 shows families of curves of the total shift  $\delta\nu(k)$  (in contrast with the curves of the normalized shift  $\delta\nu/I$  in Fig. 1) of the intensity  $I(k)$  and of the pumping efficiency  $Q(k)$  for  $a = 4$  (pumping by the line  $D_2$ ). The dashed lines here correspond to a self-absorption of the radiation with  $\kappa = 2$  and  $\kappa = 4$ .

It can be seen from a comparison with the experimental results that the calculated curves give a correct picture of the dependence of the shift on the density of the filter. Although the details (in particular, the position of the point of a zero shift) depend on the model of the spectral lineshape, the evolution of the curves (of the shift of the pumping efficiency, and of the pump intensity) upon a variation of the nitrogen density in the filter is model-independent, so it can be used as a basis for an a priori choice of the optimum nitrogen density. The best combination of small shifts and a high pumping efficiency, with an acceptable attenuation, is achieved for a filter with a Voigt parameter  $a = 3-6$  ( $P_{N_2} = 105-210$  torr). This conclusion was used in the experimental part of this study.

3. Our experimental apparatus, which had the standard layout (Ref. 6, for example), made it possible to measure the optical shifts of the frequency of the double resonance with a resolution of  $10^{-12}$  over the photocurrent range  $I_{ph} = 1-130$   $\mu A$ , which corresponds to a range  $P \approx 0.1-13$   $\mu W/cm^2$  of light flux densities. For the analysis below, it is convenient to express the intensity  $I$  in units of the relative optical broadening of the resonance:

$$I = (\gamma - \gamma_0)/\gamma_0 = (W_1 + W_2)/2\gamma_0. \quad (2)$$

The dark half-width of the resonance,  $\gamma_0$ , in a cylindrical cell with dimensions of 55 mm (the diameter) and 55 mm, filled with the mixture Ar + 0.55  $N_2$  at a total pressure of 5 torr was  $20 \pm 0.5$  Hz at the temperature  $T_C = 30^\circ C$ . As the buffer gas in the filter cell we used nitrogen at a pressure of 125 torr ( $a = 3.7$ ). The filter temperature  $T_F$  was varied over the range  $T_F = 20-100^\circ C$ . All of the measurements were carried out at two values of the temperature of the spectral lamp,  $T_L$ :  $T_L = 118^\circ C$  (corresponding to a weak self-inversion of the emission spectrum, with  $I_{ph}/I = 17$   $\mu A$  for the line  $D_1$  and 10.9  $\mu A$  for the line  $D_2$ ) and  $T_L = 141^\circ C$  (corresponding to the regime of maximum brightness, with a pronounced self-inversion;  $I_{ph}/I = 36.3$   $\mu A$  for  $D_1$  and  $I_{ph}/I = 31.4$   $\mu A$  for  $D_2$ ). The power of the rf discharge was held at the same value in all of the regimes.

Under these conditions we measured the optical shift of the resonant frequency,  $\delta\nu(I_{ph}, T_F)$ , the optical broadening  $(\gamma - \gamma_0)/I_\phi$  and the steepness of the resonance,  $g(I_\phi, T_F)$ . Comparison of the behavior  $g(I_\phi, T_F)$  with the results<sup>2)</sup> of Ref. 1 yielded an indirect determination of the shape of the  $Q(T_F)$  dependence.

The results of the measurements are shown in Figs. 3 and 4. Figure 3 shows the optical shifts  $\delta\nu(I(T_F), T_F)$  and the corresponding values of  $I(T_F)$  and  $Q(T_F)$  versus the filter temperature at  $T_L = 118^\circ C$ , for the lines  $D_1$  and  $D_2$  lines separately and also for their natural sum. The intensities  $I(T_F)$  were normalized to a unit value

at the points  $T_{F_1}$ , at which the relation  $\partial\nu/\partial T_F |_{T_{F_1}} = 0$  held.

Figure 4 shows the behavior  $\delta\nu(P_{Rb})$  for the lines  $D_1$  and  $D_2$  at  $T_L = 118^\circ C$  (solid lines) and at  $T_L = 141^\circ C$  (dashed lines). The optical density of the filter,  $k$ , is proportional to the rubidium vapor pressure  $P_{Rb}$ . Figure 4 thus allows a direct comparison with the calculated results (Fig. 2).

4. It can be seen from Figs. 1-4 that the calculations predict (and the experiments confirm) the existence of two characteristic regimes of the isotopic filtering, which occur during pumping by the lines  $D_1$  and  $D_2$  separately and also by their natural sum.

1) The first of these regimes corresponds to the choice of a filter temperature  $T_{F_0}$ , at which a change in the pump intensity is not accompanied by a change in the resonant frequency.<sup>7</sup>

2) The second regime corresponds to a filter temperature  $T_{F_1}$ , at which a small change in this temperature does not shift the resonance; i.e., we have  $\partial\nu/\partial T_F |_{T_{F_1}} = 0$ .

Which of these regimes is preferable depends on the technical capabilities in terms of stabilizing the pump intensity and the filter temperatures.

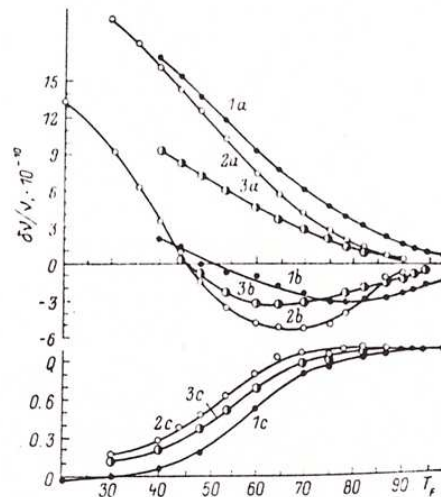


FIG. 3. 1) The line  $D_1$ ; 2) the line  $D_2$ ; 3) natural light (the sum of the lines). a - The pump intensity  $I$ ; b - the optical shift  $\delta\nu$ ; c - the pumping efficiency  $Q$ .

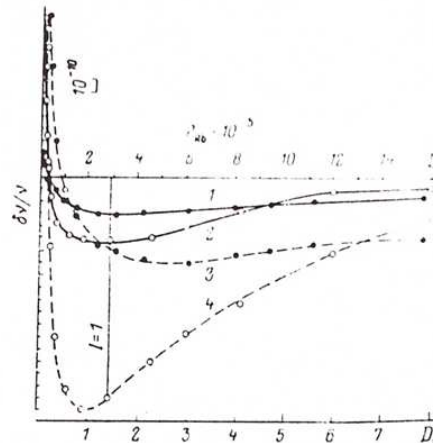


FIG. 4. Optical shift as a function of the Rb vapor pressure. 1, 3) The line  $D_1$ ; 2, 4)  $D_2$ .  $T_L$ ,  $^\circ C$ : 1, 2 - 118; 3, 4 - 141.

TABLE I

Pumping regime	$Q$	$\frac{1}{I} \frac{\partial \nu}{\partial T_F} \times 10^{-11}$	$\frac{1}{I} \frac{\partial \nu}{\partial T_L} \times 10^{-11}$	$\frac{1}{I} \frac{\partial \nu}{\partial T_C} \times 10^{-11}$	$\frac{1}{I} \frac{\partial \nu}{\partial I} \times 10^{-11}$	$\frac{1}{I} \frac{\partial \nu}{\partial T_F} \times 10^{-11}$	$\frac{1}{I} \frac{\partial \nu}{\partial T_L} \times 10^{-11}$
Line D <sub>1</sub> , T <sub>F0</sub> 50.5 °C	0.23	0	-5.2	2.6	3.1		
Line D <sub>2</sub> , T <sub>F0</sub> 45.6 °C	0.40	0	-16	-0.8	2.4	0.8	2.7
Lines D <sub>1</sub> + D <sub>2</sub> , T <sub>F0</sub> 45.6 °C	0.31	0	-16	4.0	5.6	2.9	
Line D <sub>1</sub> , T <sub>F1</sub> = 78 °C	0.90	-320	0	-16	19	1.3	3.3
Line D <sub>2</sub> , T <sub>F1</sub> = 70 °C	0.96	-530	0	-20	25	1.8	3.8
Lines D <sub>1</sub> +D <sub>2</sub> , T <sub>F1</sub> -62.5 °C	0.74	-340	0	-12	15	1.6	3.7

Note. I' satisfies the condition  $\Phi(I') = 0.1\Phi_0$ , and I'' satisfies the condition  $\Phi(I'') = 0.25\Phi_0$ .

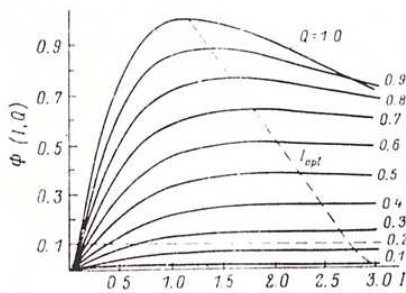


FIG. 5. The quality parameter of the 0-0 resonance versus the pump intensity I and the pumping efficiency Q.

In the first (linear) approximation, we could use the following quantity as a measure of the maximum instability caused in the resonant frequency  $\nu$  by small changes in the parameters of the system:

$$\Delta\nu(I) = \left| \frac{\partial \nu}{\partial I} \right| \Delta I + \sum_i \left| \frac{\partial \nu}{\partial T_i} \right| \Delta T_i, \quad (3)$$

where  $T_i = T_F, T_L$ , and  $T_C$ ; and the partial derivatives with respect to  $T_L$  and  $T_F$  are in turn proportional to the pump intensity I.

We know that by choosing an appropriate mixture of buffer gases in the cell we can bring the temperature coefficient of the frequency to zero (in the linear approximation) near the working point; in this case the dependence  $\nu(T_C)$  is due exclusively to cross-effects. We will be ignoring the term in (3) which contains the dependence on  $T_C$ , but we would like to point out that at optical densities of the cell which satisfy  $\alpha_0 l \gg 1$  the cross-effects can play an important role in the overall instability. For example, in our experiments  $T_L = 141^\circ\text{C}$  and  $T_C = 50^\circ\text{C}$  (a zero of the temperature coefficient of the frequency in the limit  $I \rightarrow 0$ ) we have  $1/I \partial T_C \partial \nu / \partial T_C \approx 6 \cdot 10^{-12} \text{ deg}^{-1}$ . Accordingly, all of the measurements were carried out at  $T_C = 30^\circ\text{C}$ , which corresponds to  $\alpha_0 l \approx 0.2$ .

The derivatives of the frequency with respect to the pumping parameters which appear in (3) were measured near filter temperatures  $T_F$  and  $T_{F1}$  at  $T_L = 118^\circ\text{C}$  and  $141^\circ\text{C}$ . The results are shown in Table I. We see from Fig. 4 that heating the lamp increases the optical shifts and increases

the derivatives by a factor of two to four. We will accordingly restrict the discussion below to the "cold" lamp ( $T_L = 118^\circ\text{C}$ ).

For a numerical estimate we adopt the following values for the variations in the pumping parameters:  $\Delta T_F = 0.1^\circ\text{C}$ ,  $\Delta T_L = 1^\circ\text{C}$ , and  $\Delta I = 0.01 \times I$ .

In choosing the values of the variations in the pumping parameters we allowed for the circumstance that  $\Delta T_F$  is determined by the precision at which the temperature of the constant-temperature chamber is reregulated, while the actual lamp temperature depends on this regulated temperature and the power and other properties of the rf discharge. It can vary as a result of (for example) a slow variation in the composition of the gas in the lamp or of a migration of metal along the walls of the lamp.

Note that the term  $|\partial \nu / \partial T_L| \Delta T_L$  in (3) incorporates the change in the intensity of the pump light caused by the change in  $T_L$ . Accordingly, we should understand  $\Delta I$  as representing only those changes in the intensity which are independent of the lamp conditions. Table I shows values of  $\Delta \nu(I = 1)$  corresponding to an instability of the frequency of the 0-0 resonance during pumping by light of unit intensity.

A correct comparison of pumping regimes would be carried out at a light intensity which results in a uniform sensitivity of the quantum frequency discriminator. As was shown in Ref. 1, the sensitivity or, more precisely, the quality parameter of the 0-0 resonance,  $\Phi$ , depends unambiguously on the pumping parameters in this measurement arrangement (Fig. 5):

$$\Phi(I, Q) = \frac{k^2 Q^2 I^2}{(1+I)(1+I(1+Q)) \left( 5 + \frac{1+I(1-Q)}{1+I(1+Q)} + 2 \frac{1+I(1-Q)}{1+I(1+Q)} \right)}. \quad (4)$$

Here we have used the notation in (1) and (2). It is assumed here that the noise is determined by the noise of the photocurrent.<sup>3)</sup> Clearly, the use of a regime with a larger value of Q would make it possible to substantially lower the intensity I, while maintaining the given value of the quality parameter  $\Phi(I, Q)$ .

We have used dependence (4) (Fig. 5) to

convert the values of  $\Delta\nu$  into those values of the pump intensity  $I(Q)$  which lead to the values  $\phi = 0.1\phi_0$  and  $\phi = 0.25\phi_0$  for the quality parameter in each pumping regime, where  $\phi_0$  is the maximum value of the quality parameter in the given measurement arrangement, given by

$$\phi_0 = \max_{I, Q} \phi(I, Q) = \phi(I = I_{opt}, Q = 1). \quad (5)$$

The reason for choosing such small values of  $\phi$  is that most versions of the pumping regime with  $T_F = T_{F_0}$  (Table I) are incapable of achieving large values of  $\phi$ .

5. From the results presented above we can draw the following conclusions.

1) As the lamp is heated, the specific shifts and the derivatives with respect to the pumping parameters increase sharply. Furthermore, the limiting sensitivity of the discriminator decreases, since during pumping by a self-inverting line given values of  $I$  correspond to higher values of  $I_{ph}$  and thus to a higher optical noise. Consequently, we can recommend that the spectral lamp be used at temperatures well below that corresponding to the maximum intensity in the resonant lines (23°C below that temperature in the present case).

2) Pumping by means of the line  $D_2$  leads to larger shifts than pumping by the line  $D_1$ , but in operation near in the point  $T_{F_0}$  there is a greater degree of independence from the lamp regime and a correspondingly lower instability  $\Delta\nu$ .

3) Comparison of the two filtering regimes ( $T_{F_0}$  and  $T_{F_1}$ ) at pump intensities which lead to the same values of  $\phi$  shows that the two regimes are essentially equivalent for the instabilities of the pump intensity and of the temperatures of the elements of the standard which were given above. Pumping in the line  $D_2$  in the regime  $T_F = T_{F_0}$  results in relatively smaller instabilities. It should be recalled, however, that in operation in a regime of total cancellation of the optical shift it is necessary not only to regulate the filter temperature well ( $\Delta T_F$ ) but also to achieve an accuracy in the attainment of  $T_F$  which is on the same order of magnitude. (In this regard, pumping by the line  $D_2$  is again preferable, since it makes it possible to establish  $T_F = T_{F_0}$  for essentially any value of  $T_L$ .) In operation in the regime  $T_F = T_{F_1}$ , on the other hand, there is no such restriction, and the error in the initial establishment of  $T_F$  can be  $\pm 2^\circ\text{C}$ .

4) As the buffer gas in the filter cell we recommend nitrogen at a pressure  $P_{N_2} \approx 100\text{-}200$  torr.

5) Increasing the optical density of the cell leads to a strengthening of the dependence  $\nu(T_C)$ , which stems from cross-effects. We accordingly recommend the use of cells with  $\alpha_0 l \lesssim 1$ .

6) We feel we should repeat that the values of all these optical shifts and cross-shifts which we have been discussing are directly proportional to the intensity of the pump light, so the first step to be taken toward meeting the requirement of a long-term stability of a rubidium frequency standard should be to radically reduce the intensity of the pump light, to the lowest level which provides the required short-term stability.

<sup>1)</sup>In the calculations of the shifts due to the line  $D_1$  the self-inversion of the lineshape was modeled not only by self-absorption but also through a redistribution of the intensities of the hyperfine components.

<sup>2)</sup>In the notation of (1) and (2), the expression which we used is

$$g(v) = \frac{v^2(1-v^2)}{(4+v)(4+v-v^2)},$$

where  $\frac{I}{I+1} Q$ .

<sup>3)</sup>In other words, we are treating an idealized situation here. As we pointed out in Refs. 3 and 4, the noise of the microwave field must be taken into account in the existing versions of rubidium standards. Taking this noise into account leads to a dependence which is qualitatively similar to (4) but shifted markedly down the light intensity scale, so the results presented here remain valid for real devices.

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