MAGNETIC STATE SELECTION IN ATOMIC FREQUENCY AND TIME STANDARDS

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ABSTRACT

Atomic standards such as those based upon cesium and hydrogen rely upon magnetic state selection to obtain population inversion in the hyperfine transition levels. Use of new design approaches and improved magnetic materials has made it possible to fabricate improved state selectors of small size, and thus the efficiency of utilization of beam flux is greatly improved and the size and weight of the standard is reduced. The sensitivity to magnetic perturbations is also decreased, so that the accuracy and stability of the standard is improved. Several new state selector designs are illustrated and the application to standards utilizing different atomic species is analyzed.

INTRODUCTION

The geometry and properties of the magnetic state selector are crucial elements in achieving beam standards of optimum performance. However, the overall design of the standard must be carefully considered to obtain the best balance of performance, reliability, and longevity. This paper gives a brief review of the factors which relate to the efficient utilization of beam flux and the optimization of the atomic beam state selection process, and also reviews some of the considerations which enter into the choice of atom for a standard. The design of quadrupole and hexapole state selectors is next discussed, and an idealized analysis of beam trajectories is presented for the different types. Finally, several small, efficient, magnetic state selectors are illustrated.

MAGNETIC STATE SELECTORS AND BEAM STANDARD ELEMENTS

The essential features of the atomic beam standard¹ which relate to state selectors and atomic trajectories are illustrated in Figure 1.

For beam devices designed to use velocity focussing trajectories to achieve maximum efficiency, the quadrupole or the hexapole state selector may be used, depending upon the physical properties of the particular atom. Quadrupole state selectors have a magnetic field which increases linearly with radius about the beam axis, while hexapole state selector fields increase with the square of the radius.

The source for metallic atoms is an oven, and for gasseous molecular atoms an RF discharge dissociator. The atoms emerge from the source through a collimating exit hole of large length to radius ratio to conserve flux and then pass through the state selector wherein atoms in certain magnetic quantum states are caused to converge towards the axis, while others are deflected. Atoms in the desired state pass through an interaction region to a detector in the case of magnetic resonance standards, or to a storage region within an RF cavity in the case of maser standards.

BEAM INTENSITY FACTORS

The flux utilization efficiency is the product of several factors, the most important of which are:

 $F_{1} = (Velocity Distribution)$ $F_{2} = (Source Dissociation Efficiency)$ $F_{3} = (Source Collimation Factor)$ $F_{4} = (Magnetic Hyperfine Structure of the Atom)$ $F_{5} = (State Selector Properties)$ $F_{6} = (Target Distance and Aperture)$

F₇ = (Detector Efficiency or Maser Parameters)

Figure 2 shows the normalized distribution of intensities in the beam emerging from the source as a function of velocity and temperature. For an oven source a most important consideration is that the distribution is relatively broad, and a state selector system may select atoms having considerably higher or lower velocity than the most probable, if desired. For example, in the case of cesium standards it is common practice to select velocities 50% or more lower than the peak of the distribution so as to achieve the highest line Q.

Another important result of the broad distribution is that it is not essential that the atomic state or the state selector have exact focussing properties to achieve maximum intensity, since atoms in some velocity range at a particular source emergent angle will be focussed as long as the system is only approximately idealized.

The distribution of velocities from an RF dissociator source is much less ideal than the oven source. The distribution varies with many factors such as RF power, source bulb size and material, and the degree to which thermallization occurs before emerging. The most prominent features of a discharge source are the large population of hotter than ambient atoms, and less than perfect dissociation efficiency. For a device such as the hydrogen maser the most important functions of the state selector are to capture the largest fraction of the atoms in the right state, and most importantly, to deflect strongly the wrong state atoms.

Figure 3 shows the effect of the source collimator in conserving atoms.² This gives the intensity in an increment of solid angle emerging from the source collimator as a function of the emergent angle. It is clear that a large improvement in flux utilization may be obtained with the collimator, but a peak is reached when the radius to length ratio of the collimator becomes comparable to the state selector acceptance angle. In the case of discharge sources one must be aware that recombination may occur on the collimator wall, and in practice a/L is usually no smaller than .05.

MAGNETIC HYPERFINE STRUCTURE AND FORCES ON THE ATOM

Reference (1) may be referred to for most of the theoretical basis for this paper and for the experimental data on hyperfine frequencies and other atomic and nuclear data as well as for atomic and molecular beam early history. For the purposes of trajectory analysis several approximations will be made which are entirely valid within the accuracy required. Thus the nuclear magnetic moment is considered negligible in magnitude in relation to the electronic moment, angles measured normal to the beam axis are very small so that sines equal tangents equal angles in radians, and the magnitude of the z axis velocity is equal to the total velocity magnitude.

The starting point for energy and force considerations for J = 1/2atoms, which are almost invariably the ones of concern, is the Breit-Rabi equation (Reference 1, pp 80.) The force on the atom in the radially symmetric field magnitude and field gradient of the state selector is the first derivative of the energy with respect to the radius. Figure 4 is a plot of the energy levels of an atom with nuclear moment I = 1/2 as a function of the magnetic field. The force on atoms with I greater than 1/2 and m = 0 are the same, while the forces on levels with maximum |m| are the same as for the |m| = 1levels shown. The m = 0 levels are usually the ones of primary interest for focussing in atomic standards.

For atomic beam magnetic resonance standards it is desirable to direct

atoms in a particular state through an interaction region to a relatively distant detector target. For a state with a permanent moment, or with H_1 considerably smaller than the state selector fields, a hexapole magnet provides the desired focussing fields. However, if H_1 is much greater than the state selector fields, or if some velocity dispersion is allowable in the detected atoms, the quadrupole state selector will usually provide a much more intense detected beam.

For maser standards the choice depends upon the target distance and aperture, but for the compact geometry of recent maser designs the quadrupole state selector provides very significant advantages as will be discussed later. It is seen in figure 4 that the value of H_1 for a particular atom is important in considering the dynamical behavior of the atom within the state selector. Typical quadrupole tip fields at saturation are 10 kilogauss or greater, while hexapole tip fields of 7 killogauss may be obtained.

Chart I below gives the approximate value of H_1 calculated for several interesting atoms as well as other pertinent data. The calculations for this chart use data from Reference 1.

| АТОМ | I | ν _o GHz | H1 GAUSS | ∆v/H ² -Hz/(Ga | uss) ² MULTIPLICITY |
|--------|-----|--------------------|----------|---------------------------|--------------------------------|
| H 1 | 1/2 | 1.42 | 510 | 2,750 | 4 |
| Na 23 | 3/2 | 1.77 | 630 | 2,210 | 8 |
| A1 27 | 5/2 | 1.51 | 1,610 | 290 | 12 |
| Ga 69 | 3/2 | 2.68 | 2,870 | 160 | 8 |
| Rb 85 | 5/2 | 3.04 | 1,080 | 1,290 | 12 |
| Rb 87 | 3/2 | 6.84 | 2,440 | 570 | 8 |
| Ag 107 | 1/2 | 1.71 | 610 | 2,290 | 4 |
| Ag 109 | 1/2 | 1.98 | 710 | 1,980 | 4 |
| Cs 133 | 7/2 | 9.19 | 3,280 | 430 | 16 |
| Au 197 | 3/2 | 6.11 | 2,180 | 640 | 8 |
| T1 203 | 1/2 | 21.1 | 22,600 | 20.6 | 4 |
| T1 205 | 1/2 | 21.3 | 22,800 | 20.4 | 4 |

CHART I

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In calculating beam efficiencies it is important to note that atoms with I greater than 1/2 suffer a significant loss due to the multiplicity of the states. The number of ground state hyperfine levels for each atom is listed in the last column. Not only does the multiplicity reduce the percentage of atoms in the selected state, but there are serious problems with nearby ($\Delta m = 0$) transitions which force one to use relatively high "C Fields" within the interraction region to maintain separation of the several resonances. For example, with cesium, one must use "C Fields" of the order of .04 Gauss or greater, while with I = 1/2 atoms such as thallium, silver, or hydrogen, one may use fields as low as 100 microgauss or less if desired, and there is negligible inaccuracy due to lack of knowledge of the field or due to distortions from overlapping resonances.

CURVED BORE STATE SELECTORS

To make a state selector as small as possible and to maximize the acceptance angle, the magnet bore radius should ideally be as close as possible to the beam. It is possible to make such a state selector, and in addition to achieve a focussing field for certain of the magnetic quantum states. Figure 5 illustrates the geometry of this design. The state selector may be either hexapolar or quadrupolar. It is assumed in the analysis that atoms of the largest radius are near to and have a velocity vector tangent to the bore radius. The equations defining the magnet curve are also given in Figure 5. For an atom such as thallium a strong focussing action could be obtained for the (1,0) state, while the m = 1 as well as the deflected states would be very "unfocussed." This is one example where a "pure" beam of (1,0) atoms could be obtained so that a "point" detector would not have a large noise flux of other atomic states.

In nearly all cases of interest it is not necessary (or practical) to use a curved bore state selector since the ideal bore dimensions are so small and the required curvature so slight. However, tapered bore state selectors can be made which give results nearly as good, and they are more practical to fabricate.

TAPERED BORE AND UNIFORM BORE STATE SELECTORS

Both hexapole and quadrupole state selectors with tapered bores are more efficient than uniform bore state selectors for beam resonance devices. For atoms such as hydrogen, sodium, or silver, with H₁ very much less than the magnet tip field, a hexapole magnet would be the likely choice, although for selecting very cold atoms from a higher temperature velocity distribution a relatively weak, large bore, quadrupole would be used.

In most other cases a quadrupole state selector will give the best results. It should be emphasized that for all atoms emerging from the source at a particular angle within the maximum acceptance angle there is always one velocity for which focussing occurs upon a given target. Thus if the range of focussed velocities falls within the more probable part of the velocity distribution, a very efficient selection of the desired state may be obtained. For most atoms a quadrupole state selector may be configured to obtain the best results, even though H_1 is only a fraction of the magnet tip field.

Figure 6 diagrams the coordinates and defines the parameters which are used in subsequent equations for both the tapered bore and the constant bore state selectors. (For constant bore $\alpha = 0$) θw^2 is defined by the ratio of maximum potential energy the atom incurs in traversing the field from the axis to the bore tip divided by the thermal kinetic energy. It should be noted that the thermal kinetic energy of the atom in the beam, $1/2mv^2$, is equal to 3/2 KT, and is independant of the particular atomic mass. It is assumed the state selector tip iron is saturated and the tip field is constant.

Figure 7 gives the trajectory equations for the quadrupole state selector for states which have a constant magnetic moment or in which the moment is essentially constant due to the magnet fields being generally greater than H_1 . Figure 8 gives the results for other cases noted therein.

The equations given in the figures, if used with judgement, provide a good basis for approximating the best state selector type, as well as the bore radius and length, for a particular atom and detector target aperture and distance.

If desired, the equations of motion may be solved exactly for all cases. Thus, if Ww is the magnetic potential energy (derived from the Breit-Rabi equation), the differential equation to be solved is:

$$m\ddot{r} \pm \frac{\partial W_{m}}{\partial r} = 0$$
,

which solves immediately for the angle $\theta = dr/dz$:

$$\Theta^2 = \Theta_0^2 \neq \frac{W_w}{\left(\frac{1}{2}mv^2\right)} \cdot$$

From here r may be solved for by elementary means for either the hexapole or quadrupole.

The accuracy achieved by exact computation usually far exceeds the practical necessity in view of the uncertainties due to mechanical tolerances of the state selector, alignment inaccuracies, or the imperfection of the magnetic field pattern. Several papers on beam calculation methods have been published, one of which is given in Reference 3.

STATE SELECTORS FOR HYDROGEN MASERS

The hydrogen maser and similar devices present a different problem than beam resonance devices. Traditionally, masers used hexapole state selectors which were placed a relatively large distance from the bulb, and were designed to focus atoms near the peak of the modified Maxwellian velocity distribution. This system is quite inefficient due to the small solid angle the bulb entrance subtends and the loss of the atoms in the higher temperature part of the real velocity distribution.

A quadrupole with very small bore diameter, and length to radius ratio much greater than that dictated by the peak of normal velocity distribution, will "capture" the largest possible flux of atoms from a source. Due to its small size and the small level of stray fields caused by the magnet, it may be placed within 1 cm or less of the maser shields without incurring shielding problems. Thus the state selector to bulb distance can be minimized. Typical state selector entrance maximum capture angles are .04 radians or less (much less for higher velocity atoms) thus if the bulb distance is 2 inches, a bulb entrance diameter of .16 inches will "capture" essentially all of the atoms "captured" in the state selector. Most importantly though, an atom which is in a state to be deflected and which starts out with a zero entrance angle will have a relatively large exit angle. Calculations for the small magnet indicate that essentially all of the "wrong state" atoms will not enter the bulb in the above example.

Due to the high state selection efficiency of the small quadrupole in a compact maser design, the source exit collimator diameter may be very small, and the idealization assumed in the calculations that the atom enters the state selector from a point source is closely realized. Hydrogen atom flux efficiencies 1,000 times better than obtained with early hydrogen masers are thus possible with recent maser designs.^{4,5}

STATE SELECTOR DESIGNS

Figure 9 is a picture showing 3 state selectors recently made at Sigma Tau Standards Corporation which are examples of the state of the art at this writing. On the left is a tapered bore quadrupole with a bore entrance diameter of .30 mm, exit diameter 1.4 mm, length 38 mm, and $\alpha = .0145$.

On the right in Figure 9 is a tapered bore hexapole with entrance diameter .90 mm, exit diameter 1.70 mm, length 38 mm and α = .011.

In the center in Figure 9 is a very small tapered bore quadrupole with entrance diameter .46 mm, exit diameter .97 mm, length 25.4 mm and $\alpha = .010$. This state selector has been designed for a high flux compact hydrogen maser. The maximum diameters that may be used with this small state selector and still maintain magnetic saturation is

about 1.2 mm and the minimum, dictated by present mechanical tolerances, is about .25 mm. Within this range and with a length of 25.4 mm (1 inch) it may easily be configured to the requirements of atomic beam resonance standards using many of the different atoms described in this paper. The particular dimensions of the small state selector shown in Figure 9 are ideal for compact hydrogen masers with state selector to bulb distances of 2 inches to 8 inches or over, depending upon bulb aperture.

CONCLUSION

This paper illustrates that with new state selector designs and new and improved atomic beam standard configurations it is possible to achieve much more efficient use of source flux and to focus very large intensities of a variety of atoms. It is thus very possible to improve the efficiency, stability, and accuracy of existing standards or to design new standards based upon atoms which have fundamental properties which may be superior to those of standards presently in use.

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Figure 2. Intensity Distribution Of Atoms In A Beam Emerging From An Oven Or Discharge Source.



Figure 3. Intensity Of Beam In An Increment Of Solid Angle Emerging From A Source Collimator Versus The Emergent Angle.



Figure 4. Magnetic Hyperfine Energy Levels Of An Atom With J = 1/2 And I = 1/2 Versus Magnetic Field.







Figure 6. Diagram Of Coordinates And Parameters For Analysis Of Atom Trajectories Within State Selectors.

ATOM PATH IN QUADRUPOLE STATE SELECTOR FOR F(1,±1) STATES OR F($\frac{1}{0}, \frac{0}{0}$) WITH H>H, $r_0 = 0$, $R = R_0 + \propto Z$, $\Theta_r^2 = \frac{M_0 H}{(2m_1 Z^2)} = \Theta_u^2$ $\frac{J^2 r}{JZ^2} + \frac{\Theta_r^2}{ZR} = 0$ (+ATTRACTING) $r = \Theta_0 Z = \frac{\Theta_r^2}{Z \propto 2} \left[R \left\{ f_n(\frac{R}{R_0}) - I \right\} + R_0 \right]$ $\Theta = \Theta_0 Z = \frac{\Theta_r^2}{Z \propto 2} \left[R \left\{ f_n(\frac{R}{R_0}) - I \right\} + R_0 \right]$ $AS \propto 0$ (NO TAPER) $r = \left(\Theta_0 Z = \frac{\Theta_r^2 Z}{4 R_0}\right) Z$, $\Theta = \Theta_0 Z = \frac{\Theta_r^2 Z}{2R_0}$

Figure 7. Equations Of Motion Within State Selector For Cases Where The Magnetic Moment Is Constant, Or Nearly So. ATOM PATH IN QUADRUPOLE STATE SELECTOR FOR F(1,0/0,0) STATES (H<H,) OR HEXAPOLE FOR $F(1,\pm 1)$ STATES. $f_0 = O$, $R = R_0 + \propto =$

 $\begin{aligned} & \Theta_{W}^{2} = \frac{g_{T}H\Theta_{T}^{2}}{4H_{I}} \left(H < H_{I}, F(I, O/O, O)\right) \\ & \Theta_{W}^{2} = \Theta_{T}^{2} = \frac{M_{0}H_{I}}{(2M_{N}T_{T})} \left(H > H_{I}, or F(I, \pm I)\right) \\ & \text{ATTRACTING:} \qquad \Phi_{I} \equiv B_{I} lm_{R_{0}}^{R} \right), \quad B_{I} \equiv \int_{\Theta_{T}}^{\Theta_{T}} -\frac{1}{4} \\ & r = \frac{\Theta_{0} \sqrt{RR_{0}} \propto}{B_{I}} SIN \left(\Phi_{I}, \Phi\right) = \frac{\Theta_{0} \sqrt{RR_{0}}}{2B_{I}} \left[SIN \Phi_{I} + 2B_{I} Cos \Phi_{I}\right] \\ & \text{DEFLECTING: Replace Sin With Sinh, Cos With Cosh} \\ & \mathcal{A} = B_{2} ln (B_{R_{0}}), \quad B_{2} \equiv \int_{\Theta_{T}}^{\Theta_{T}} +\frac{1}{4} \\ & LIM \propto \to O \quad ATT: \quad \Gamma = \Gamma_{MAX} SIN \Phi_{3}, \quad \Theta = \Theta_{0} Cos \Phi_{3} \\ & \Phi_{3} \equiv \Theta_{W} \frac{Z}{R_{0}} \quad DEF: \quad \Gamma = \Gamma_{L} M_{X} SIN h \Phi_{3}, \quad \Theta = \Theta_{0} Cosh \Phi_{3} \end{aligned}$

Figure 8. Equations Of Motion Within Quadrupole State Selector For (m = 0) Cases Where H Is Less Than H₁ Or Within Hexapole In Cases Where The Magnetic Moment Is Constant, Or Nearly So.



Figure 9. Quadrupole And Hexapole State Selectors Produced At Sigma Tau Standards Corporation. For Dimensional Reference The Small Quadrupole In The Center Has A Tapered Bore With Entrance Diameter of .46 mm, Exit Diameter .97 mm, And Is 25.4 mm Long. The Poles Are Saturated And Have Tip Fields Of Approximately 10 Kilogauss In The Quadrupole Units, And 7 Kilogauss In The Hexapole.