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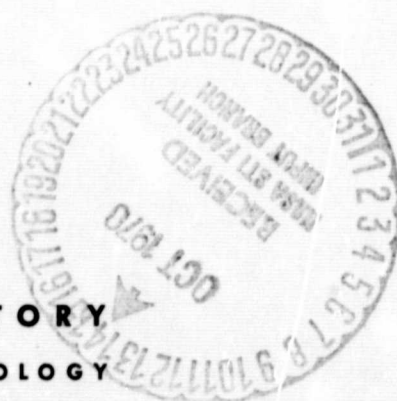
Technical Memorandum 33-456

*Comparative Performance of Double Focused and
Quadrupole Mass Spectrometers*

S. K. Wilson

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JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CALIFORNIA

September 1, 1970

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Quadrupole Mass Spectrometers***

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National Aeronautics and Space Administration

Preface

The work described in this report was performed by the Space Sciences Division of the Jet Propulsion Laboratory.

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Abstract

A comparison is made of double focused and quadrupole mass spectrometers by analytical means. The analysis considers size, weight, and power for both types of instruments at identical resolutions and sensitivity for the same mass number. In the analysis, both instruments are used with equivalent ion sources having a 10-V voltage spread. It is shown that with weight and power the bases for comparison, the double-focused mass spectrometer is the better.

Comparative Performance of Double Focused and Quadrupole Mass Spectrometers

I. Introduction

This analysis is for the purpose of comparing the performance of the double focused quadrupole models of flight-type mass spectrometers. They are compared in size, weight, and power for the same resolution at the same mass number. In addition, the voltage, mechanical stability, and the effects of space charge are compared.

The size, weight, and power comparison is based on the conditions of equal source area and sensitivity variations of not more than 40% over the mass range.

II. Basic Relationships

A. Double-Focused Spectrometer

The basic transfer function for the double focused mass spectrometer, using linear analysis, is given by

$$\begin{bmatrix} \dot{X}_{mc} \\ X_{mc} \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{\ell_{mc}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos \theta_M & -\dot{\theta}_M \sin \theta_M & 0 \\ \frac{\sin \theta_M}{\dot{\theta}_M} & \cos \theta_M & 1 \\ 0 & 0 & 0 \end{bmatrix} \left\{ \begin{bmatrix} 1 & 0 & 0 \\ \frac{\ell_{em}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & -2^{1/2} \dot{\theta}_e \sin 2^{1/2} \theta_e & 0 \\ \frac{\sin 2^{1/2} \theta_e}{2^{1/2} \dot{\theta}_e} & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix} \right.$$

$$\times \left\{ \begin{bmatrix} v_m \sin \alpha \\ X_0 + \ell_e \tan \alpha \\ 0 \end{bmatrix} + r_e \beta_e \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\} + r_m \beta_m \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \Bigg\}$$

where

l_{mc} = distance from the magnetic sector to the collector slit

l_{em} = distance between the electric sector to the magnetic sector

l_e = distance between the object slit and the electric sector

θ_m = angle of rotation for the ions while they are in the magnetic field

θ_e = angle of rotation in the electric sector

β_e = velocity dispersion in the electric sector

β_m = velocity dispersion in the magnet sector

$\dot{X}_{mc}$ = the transverse velocity at the collector slit

X_{mc} = displacement from the optic axis at the collector slit

v_m = velocity of the ions which travel along the optic axis

α = the initial angle between the paths of an ion and the optic axis

r_e = radius of the optic axis in the electric sector

r_m = radius of the optic axis in the magnetic sector

Each sector has an object and image distance. The image distance is related to the object distance by the following:

Electric Sector

$$\left[\frac{l_{ei}}{v_m} \quad 1 \right] \begin{bmatrix} \cos 2^{1/2} \theta_e & -2^{1/2} \frac{v_m}{r_e} \sin 2^{1/2} \theta_e \\ \frac{\sin 2^{1/2} \theta_e}{\theta_e} & \cos 2^{1/2} \theta_e \end{bmatrix} \begin{bmatrix} v_m \\ l_e \end{bmatrix} = 0$$

$$\tan 2^{1/2} \theta_e = \frac{\frac{l_{ei}}{r_e} + \frac{l_e}{r_e}}{\frac{2^{1/2} l_{ei} l_e}{r_e^2} - \frac{1}{2^{1/2}}}$$

If

$$l_{ei} = l_e$$

then

$$\frac{l_e}{r_e} = \frac{1}{2^{1/2}} \frac{(1 + \cos 2^{1/2} \theta_e)}{\sin 2^{1/2} \theta_e} \quad (\text{symmetric case})$$

Magnetic Sector

$$\left[\frac{l_{mc}}{v_m} \quad 1 \right] \begin{bmatrix} \cos \theta_m & -\frac{v_m}{r_m} \sin \theta_m \\ \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m \end{bmatrix} \begin{bmatrix} v_m \\ l_e \end{bmatrix} = 0$$

$$\tan \theta_m = \frac{\frac{l_{im}}{r_m} + \frac{l_{mc}}{r_m}}{\frac{l_{im} l_{mc}}{r_m^2} - 1}$$

If

$$l_{im} = l_{mc}$$

$$\frac{l_{mc}}{r_m} = \frac{1 + \cos \theta_m}{\sin \theta_m} \quad (\text{symmetric case})$$

where

l_e = object distance for the electric sector

l_{ei} = image distance for the electric sector

l_{im} = object distance for the magnetic sector

l_{mc} = image distance for the magnetic sector

$l_{em} = l_{ei} + l_{im}$

The magnification is given by

$$G = G_e G_m$$

Electric Sector

$$G_e = \left[\frac{l_{ei}}{v_m} \quad 1 \right] \begin{bmatrix} \cos 2^{1/2} \theta_e & -2^{1/2} \frac{v_m}{r_e} \sin 2^{1/2} \theta_e \\ \frac{r_e}{2^{1/2} v_m} \sin 2^{1/2} \theta_e & \cos 2^{1/2} \theta_e \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= \frac{-2^{1/2} l_{ei}}{r_e} \sin 2^{1/2} \theta_e + \cos 2^{1/2} \theta_e$$

$$= -1 \quad (\text{symmetric case})$$

$$\frac{l_{ei}}{r_e} = \frac{\cos 2^{1/2} \theta_e - G_e}{2^{1/2} \sin 2^{1/2} \theta_e}$$

$$\frac{l_e}{r_e} = \frac{\cos 2^{1/2} \theta_e - 1/G_e}{2^{1/2} \sin 2^{1/2} \theta_e}$$

Magnetic Sector

$$G_m = \begin{bmatrix} \frac{l_{mc}}{v_m} & 1 \end{bmatrix} \begin{bmatrix} \cos \theta_m & \frac{-v_m}{r_m} \sin \theta_m \\ \frac{r_m \sin \theta_m}{v_m} & \cos \theta_m \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= -\frac{l_{mc}}{r_m} \sin \theta_m + \cos \theta_m$$

$$= -1 \text{ (symmetric case)}$$

$$\frac{l_{mc}}{r_m} = \frac{\cos \theta_m - G_m}{\sin \theta_m}$$

$$\frac{l_{im}}{r_m} = \frac{\cos \theta_m - \frac{1}{G_m}}{\sin \theta_m}$$

The conditions for a velocity focus are

$$X_{mc} = 0$$

when

$$\beta_e = \beta_m \neq 0$$

$$X_o = 0$$

$$\alpha = 0$$

$$X_{mc} = \begin{bmatrix} \frac{l_{mc}}{v_m} & 1 & 0 \end{bmatrix} \begin{bmatrix} \cos \theta_m & \frac{-v_m}{r_m} \sin \theta_m & 0 \\ \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m & 1 \\ 0 & 0 & 0 \end{bmatrix} \left\{ \begin{bmatrix} 1 & 0 & 0 \\ \frac{l_{em}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & \frac{-2^{1/2} v_m \sin \theta_e}{r_e} & 0 \\ \frac{r_e \sin 2^{1/2} \theta_e}{2^{1/2} v_m} & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix} r_e \beta_e \right.$$

$$\times \left\{ \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} r_m \beta_m + \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\}$$

$$= \begin{bmatrix} \frac{l_{mc}}{v_m} & 1 & 0 \end{bmatrix} \begin{bmatrix} \cos \theta_m & -v_m \sin \theta_m & 0 \\ \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m & 1 \\ 0 & 0 & 0 \end{bmatrix} \left\{ \begin{bmatrix} 0 & 0 & 0 \\ \frac{l_{ei}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & -2^{1/2} \frac{v_m}{r_e} \sin 2^{1/2} \theta_e & 0 \\ \frac{r_e}{2^{1/2} v_m} \sin 2^{1/2} \theta_e & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix} r_e \beta_e \right.$$

$$\times \left\{ \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} + r_m \beta_m \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} \right\}$$

$$X_{mc} = \beta_e G_m r_e (1 - G_e) + \beta_m r_m (1 - G_m)$$

If

$$\beta_e = \beta_m$$

$$X_{me} = 0$$

$$G_m r_e (1 - G_e) + r_m (1 - G_m) = 0$$

$$\frac{r_e}{r_m} = \frac{1 - 1/G_m}{(1 - G_e)}$$

If

$$G_e = -1$$

$$\boxed{\frac{r_e}{r_m} = \frac{1 - 1/G_m}{2}}$$

If

$$\begin{aligned} G_e &= -1 \\ G_m &= -1 \end{aligned} \quad \left(\begin{array}{l} \text{symmetric, electric,} \\ \text{and magnetic sectors} \end{array} \right)$$

then

$$r_e = r_m$$

The displacement in the electric sector is given by

$$y_e = \begin{bmatrix} \frac{r_e \sin 2^{1/2} \theta_e}{2^{1/2} v_m} & \cos 2^{1/2} \theta_e & 1 \end{bmatrix}$$

$$\times \left\{ \begin{bmatrix} v_0 \sin \alpha \\ X_0 + l_e \tan \alpha \end{bmatrix} + r_e \beta_e \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\}$$

$$= \left(\frac{r_e^2}{2} \sin^2 \alpha + (X_0 + l_e \tan \alpha - r_e \beta)^2 \right)^{1/2}$$

$$\times \sin 2^{1/2} (\theta_e + \phi_e) + r_e \beta$$

where

$$\tan 2^{1/2} \phi_e = 2^{1/2} \frac{(X_0 + l_e \tan \alpha - r_e \beta)}{r_e \sin \alpha}$$

$$|X_e|_{\max} = \left(\frac{r_e^2}{2} \sin^2 \alpha + (X_0 + l_e \tan \alpha - r_e \beta)^2 \right)^{1/2} + \beta r_e$$

The displacement in the magnetic sector is given by

$$X_m = \begin{bmatrix} \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m & 1 \end{bmatrix} \left\{ \begin{bmatrix} 1 & 0 & 0 \\ \frac{l_{em}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & \frac{-2^{1/2} v_m}{r_e} \sin 2^{1/2} \theta_e & 0 \\ \frac{r_e}{2^{1/2} v_m} \sin 2^{1/2} \theta_e & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix} \right\}$$

$$\times \left\{ \begin{bmatrix} v_m \sin \alpha \\ X_0 + l_e \tan \alpha \\ 0 \end{bmatrix} + r_e \beta_e \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} + r_m \beta_m \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\}$$

$$X_m = \begin{bmatrix} \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m & 1 \end{bmatrix} \left\{ \begin{bmatrix} 0 & 0 & 0 \\ \frac{l_{ei}}{v_m} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & \frac{-2^{1/2}}{r_e} v_m l_{im} 2^{1/2} \theta_e & 0 \\ \frac{r_e}{2^{1/2} v_m} \sin 2^{1/2} \theta_e & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ X_0 \\ 0 \end{bmatrix} + r_e \beta_e \right\}$$

$$\times \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \left\{ + r_m \beta_m \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\} + \begin{bmatrix} 1 & 0 & 0 \\ \frac{\ell_{im}}{v_m} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos 2^{1/2} \theta_e & \frac{-2^{1/2} v_m}{r_e} \sin 2^{1/2} \theta_e & 0 \\ \frac{r_e}{2^{1/2} v_m} \sin 2^{1/2} \theta_e & \cos 2^{1/2} \theta_e & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\times \left\{ \begin{bmatrix} v_m \sin \alpha \\ X_0 + \ell_e \tan \alpha \\ 0 \end{bmatrix} + r_e \beta_e \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \right\}$$

$$X_m = \sin(\theta_m + \phi_m) \left\{ (-2^{1/2} X_0 - r_m \sin \alpha + \beta 2^{1/2} r_m \sin 2^{1/2} \theta_e)^2 + \left[\ell_{im} \sin \alpha + X_0 \left(\frac{\ell_{im}}{r_m} 2^{1/2} \sin 2^{1/2} \theta_e - 1 \right) \right. \right. \\ \left. \left. + \beta (r_m + \ell_{im} 2^{1/2} \sin 2^{1/2} \theta_e) \right]^2 \right\}^{1/2} + r_m \beta$$

where

$$\tan \phi_m = \frac{\ell_{im} \sin \alpha + X_0 (\ell_{im} 2^{1/2} \sin 2^{1/2} \theta_e - 1) + \beta (r_m + \ell_{im} 2^{1/2} \sin 2^{1/2} \theta_e)}{-2^{1/2} X_0 - r_m \sin \alpha + \beta 2^{1/2} r_m \sin 2^{1/2} \theta_e}$$

$$|X_m|_{\max} = \left((-2^{1/2} X_0 - r_m \sin \alpha + \beta 2^{1/2} r_m \sin 2^{1/2} \theta_e)^2 + \left[\ell_{im} \sin \alpha + X_0 \left(\frac{\ell_{im}}{r_m} 2^{1/2} \sin 2^{1/2} \theta_e - 1 \right) \right. \right. \\ \left. \left. + \beta (r_m + \ell_{im} 2^{1/2} \sin 2^{1/2} \theta_e) \right]^2 \right)^{1/2} + \beta r_m$$

The ionic path length along the optic axis is given by

Electric Sector

$$\frac{Y_e}{r_e} = \theta_e + (\ell_e + \ell_{ei})/r_e$$

$$= \theta_e + \frac{\left(-\frac{1}{G_e} - G_e + 2 \cos 2^{1/2} \theta_e \right)}{2^{1/2} \sin 2^{1/2} \theta_e}$$

For the symmetric case

$$G_e = -1$$

$$\frac{Y_e}{r_e} = \theta_e + \frac{2^{1/2} (1 + \cos 2^{1/2} \theta_e)}{\sin 2^{1/2} \theta_e}$$

Magnetic Sector

$$\frac{Y_m}{r_m} = \theta_m + (\ell_{im} + \ell_{me})/r_m$$

$$= \theta_m + \frac{\left(-\frac{1}{G_m} - G_m + 2 \cos \theta_m \right)}{\sin \theta_m}$$

For the symmetric case

$$G_m = -1$$

$$\frac{Y_m}{r_m} = \theta_m + \frac{2(1 + \cos \theta_m)}{\sin \theta_m}$$

The total ionic path length is given by

$$Y_t = Y_e + Y_m$$

For the symmetric sectors

$$\frac{Y_t}{r_m} = \theta_e + \theta_m + \frac{2(1 + \cos \theta_m)}{\sin \theta_m} + \frac{2(1 + \cos 2^{1/2} \theta_e)}{2^{1/2} \sin 2^{1/2} \theta_e}$$

The mass dispersion is given by

$$\begin{aligned} D_m &= \frac{X_{mc}}{r_m} = \beta_m \begin{bmatrix} \frac{l_{mc}}{v_m} & 1 & 0 \end{bmatrix} \begin{bmatrix} \cos \theta_m & \frac{-v_m}{r_m} \sin \theta_m & 0 \\ \frac{r_m}{v_m} \sin \theta_m & \cos \theta_m & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \\ &= \beta_m \begin{bmatrix} \frac{l_{mc}}{v_m} & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{v_m}{r_m} \sin \theta_m \\ 1 - \cos \theta_m \end{bmatrix} \\ &= \beta_m \left[\frac{l_{mc}}{r_m} \sin \theta_m + 1 - \cos \theta_m \right] \\ \beta_m &= \frac{\Delta v}{v} \\ &= -\frac{1}{2} \frac{\Delta m}{m} \\ |D_m| &= \frac{1}{2} \frac{\Delta m}{m} (1 - G_m) \end{aligned}$$

For the symmetric case

$$|D_m| = \frac{\Delta m}{m}$$

$$= \frac{\frac{1}{2}(1 - G_m)r_m}{X_s + X_0 G}$$

The dispersion that would allow a mass range Δm to be transmitted through the exit slit is given by

$$\boxed{\frac{m}{\Delta m} = \frac{\frac{1}{2}(1 - G_m)r_m}{X_s + X_0 G_e G_m}}$$

$$D_m r_m = X_s + X_0 G$$

If

where X_s is the exit slit width

$$X_s = X_0$$

and

$$G_e = -1$$

$$\frac{m}{\Delta m} = R$$

$$= \frac{\frac{1}{2}(1 - G_m)}{|D_m|}$$

$$\boxed{\frac{m}{\Delta m} = \frac{1}{2} \frac{r_m}{X_0}}$$

B. Quadrupole Spectrometer

The force equations for the quadrupole mass spectrometer are:

$$m\ddot{x} + \frac{2e}{r_0^2} (V_\omega \cos \omega t + V_D) X = 0$$

$$m\ddot{y} - \frac{2e}{r_0^2} (V_\omega \cos \omega t + V_D) y = 0$$

These equations can be transformed to give

$$\frac{d^2 X}{d\tau^2} + (a + 2q \cos 2\tau) X = 0$$

$$\frac{d^2 y}{d\tau^2} - (a + 2q \cos 2\tau) y = 0$$

where

$$a = \frac{8eV_D}{r_0^2 m \omega^2}$$

$$q = \frac{4eV_\omega}{r_0^2 m \omega^2}$$

$$\tau = \frac{\omega t}{2}$$

The first stability zone for the quadrupole is given by

$$0 < q < 0.92$$

$$0 < \gamma < 0.166$$

where

$$\gamma = \frac{V_D}{V_\omega}$$

The resolution is given by the following:

$$\frac{m}{\Delta m} = \frac{0.75}{1 - \frac{\gamma}{\gamma_{\max}}}$$

The ions must be in the dynamic field for a number of cycles n before they can be resolved

$$n \geq 3.5 \left(\frac{m}{\Delta m} \right)^{1/2}$$

The maximum entry radius for parallel rays that would allow transmission is given by

$$r_i = \frac{r_0}{2.7 \left(\frac{m}{\Delta m} \right)^{1/2}}$$

The maximum entry angle, at $r_i = 0$, which would allow transmission is given by

$$\tan \theta_0 = \frac{\left(\frac{V_\omega}{V_z} \right)^{1/2}}{2.5 \left(\frac{m}{\Delta m} \right)^{1/2}}$$

V_z = Axial energy of the ions

C. Focused-Beam Transmission Through an Aperture

When a beam of charged particles is demagnified and focused on an aperture, the thermal energies of the particles establish a limit to the amount of current that is transmitted. The current density at the image plane is given by

$$J_0 = J_s [1 - (1 - \beta^2) \exp -\beta^2 \Phi / (1 - \beta^2)] / G^2$$

where

J_s = current density at the ionization plane

$$\beta = G \sin \theta$$

G = magnification

θ = maximum angle that the ions can have with respect to the optic axis at the image plane

$$\Phi = \frac{eV}{kT}$$

V = potential at the image plane

e = electronic charge

k = Boltzmann's constant

T = absolute temperature

The limit of this expression, as $G \rightarrow 0$, is given by

$$J_0 = J_s (1 + \Phi) \sin^2 \theta$$

The magnification factor producing a current density that is 63.3% of the maximum is given by

$$G = \frac{1}{\left(\frac{eV}{kT}\right)^{1/2} \sin \theta}$$

If

$$G^2 \sin^2 \theta \ll 1$$

The demagnification factor is given by

$$G = \left(\frac{A_0}{A_s}\right)^{1/2}$$

where

A_0 = area of the objective aperture

A_s = cross sectional area of the ion beam at the ionization plane

$$\left(\frac{eV}{kT}\right) \sin^2 \theta = \frac{A_s}{A_0}$$

The current density for an aperture that is a rectangular slit is given by

$$J_0 = J_s \left[\operatorname{erf}(\beta^2 \phi / (1 - \beta^2))^{1/2} + \beta e^{\Phi} [1 - \operatorname{erf}(\Phi / (1 - \beta^2))^{1/2}] \right] / G$$

where $\operatorname{erf} x$ is equal to

$$\frac{2}{\pi^{1/2}} \int_0^x \exp -u^2 du$$

The limit for this expression, for $G \rightarrow 0$ is given by

$$J_0 = J_s \frac{2}{\pi^{1/2}} \left(\frac{eV}{kT}\right)^{1/2} \sin \theta$$

since

$$\operatorname{erf} x \simeq \frac{2}{\pi^{1/2}} x$$

when

$$x \ll 1$$

If

$$X = 1$$

$$\operatorname{erf} X = 0.84$$

$$G \sin \theta \ll 1$$

$$G = \frac{1}{\sin \theta \Phi^{1/2}}$$

$$J_0 = J_s (0.84) \left(\frac{eV}{kT}\right)^{1/2} \sin \theta$$

This value of current density is 74.5% of the maximum value. The magnification factor for this case is given by

$$G = \frac{A_0}{A_s} = \frac{1}{\sin \theta \Phi^{1/2}}$$

Therefore,

$$\left(\frac{eV}{kT}\right)^{1/2} \sin \theta = \frac{A_s}{A_0}$$

D. Field-Free Transmission Through a Channel

The thermal distribution is given by

$$dn = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp -mv_z^2/2kT dv_z$$

$$v_z = v_m \tan \alpha_z$$

$$v_m = r_m \frac{Be}{m} \quad (\text{magnetic sector})$$

$$dn = \frac{r_m Be}{(2\pi mkT)^{1/2}} \exp \left(\frac{-r_m^2 e^2 B^2 \tan^2 \alpha_z}{2mkT} \right) d \tan \alpha_z$$

Let

$$u = \left(\frac{m}{kT}\right)^{1/2} v_z$$

$$= r_m Be \tan \alpha_z / (mkT)^{1/2}$$

$$n = \frac{1}{(2\pi)^{1/2}} \int_{u_1}^{u_2} \exp -u^2/2 du$$

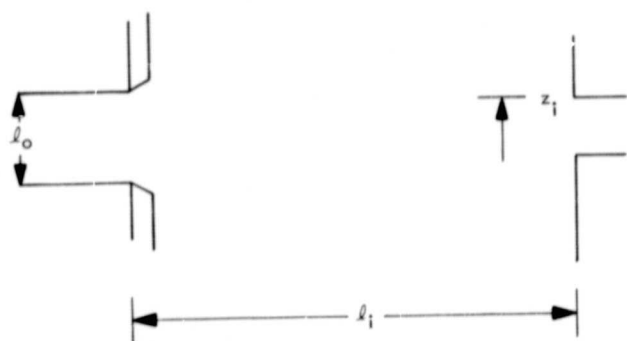
where n is the particle density which is assumed to be uniform over the object slit.

The relative transmission is given by

$$T_r = \int \frac{ndz}{\ell_0}$$

where ℓ_0 is the length of the object slit.

$$T_r = \frac{1}{\ell_0 (2\pi)^{1/2}} \int_{-\ell_0/2}^{\ell_0/2} \int_{u_1}^{u_2} e^{-u^2/2} du dz$$



$$\tan \alpha_{z,1} = \frac{z_i - z}{\ell_i}$$

$$\tan \alpha_{z,2} = \frac{-z_i - z}{\ell_i}$$

$$u_1 = \left(\frac{m}{kT} \right)^{1/2} v_m \tan \alpha_{z,1}$$

$$u_2 = \left(\frac{m}{kT} \right)^{1/2} v_m \tan \alpha_{z,1}$$

The transmission efficiency is more than 84% when

$$u/2^{1/2} \geq 1$$

since

$$\frac{2}{\pi} \int_0^1 \exp -x^2 dx = 0.8427$$

$$\left| \frac{z_i - \frac{\ell_0}{2}}{\ell_i} \right| = |\tan \alpha_{z,1}| \geq \frac{2^{1/2}}{v_m} \left(\frac{kT}{m} \right)^{1/2}$$

$$\frac{|z_i - \ell_0/2|}{\ell_i} \geq \frac{2^{1/2}}{v_m} \left(\frac{kT}{m} \right)^{1/2}$$

$$\ell_0 = 4z_i$$

Since the same criteria can be used for a point source with $\ell_0 = 0$ so that

$$z_i \geq \frac{\ell_i 2^{1/2} \left(\frac{kT}{m} \right)^{1/2}}{v_m}$$

$$= \ell_i \left(\frac{kT}{eV_m} \right)^{1/2}$$

E. Statically-Focused Beam Transmission Through a Channel

When z -axis focusing is used, 74.5% transmission is possible when

$$G^2 \sin^2 \alpha_z \frac{eV_m}{kT} = 1 - G^2 \sin^2 \alpha_z$$

$$G = \frac{2z_i}{\ell_0}$$

$$\tan \alpha_z = \frac{\ell_0/2}{\ell_i}$$

$$G \simeq \frac{1}{\sin \alpha_z} \left(\frac{kT}{eV_m} \right)^{1/2}$$

$$z_i \simeq \frac{\ell_0}{2 \sin \alpha_z} \left(\frac{kT}{eV_m} \right)^{1/2}$$

$$\simeq \ell_i \left(\frac{kT}{eV_m} \right)^{1/2}$$

F. Magnet Size

It is assumed that the cross-sectional area of the magnet is equal to the cross-sectional area of the magnetic analyzer.

$$L_m H_m = f_1 \ell_g B$$

$$A_m B_m = f_2 A_g B$$

$$A_m = A_g$$

$$B = \frac{B_m}{f_2}$$

$$\frac{L_m}{\ell_g} = \frac{f_1}{f_2} \frac{B_m}{H_m}$$

where

L_m = length of the magnet

A_m = area of the magnet

ℓ_g = length of the air gap

A_g = area of the air gap

f_1 = mmF leakage factor

f_2 = flux leakage factor

H_m = field intensity of the magnet

B_m = flux density of the magnet

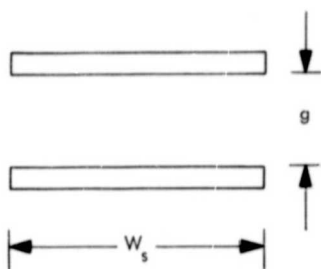
G. Width of the Sectors

g_s = spacing between parallel boundaries

W_s = width of the boundaries

$$\frac{W_s}{g_s} \geq 6$$

This limit is necessary to prevent excessive fringing and to provide a homogenous magnetic and/or electric field.



H. Rod Capacitance

The static potential between the rod pairs is given by

$$V = \frac{V_0 (y^2 - x^2)}{r_0^2}$$

The capacitance is given by

$$C = \frac{\epsilon_0 \int E \cdot ds}{\int E \cdot dl}$$

$$E = \frac{2V_0}{r_0^2} (ix - jy)$$

$$|E| = \frac{2V_0}{r_0^2} (x^2 + y^2)^{1/2}$$

$$= \frac{2V_0}{r_0^2} \left(1 + \frac{y^2}{x^2} \right)^{1/2} x$$

$$ds = L (idx + jdy)$$

$$= L \left(1 + \frac{dy}{dx} \right)^{1/2} dx$$

L = length of the rods

Integrating along the line $x = y$,

$$ds = L 2^{1/2} dx$$

$$\int_0^{r_0} E \cdot dl = V_0$$

$$C = \frac{4\epsilon_0}{r_0^2} \int_0^{r_0} L 2^{1/2} x 2^{1/2} dx$$

$$= 4\epsilon_0 L$$

ϵ_0 = permittivity of free space

I. Power Consumption in a Dynamic Field

The average energy that is stored in an electric field is given by

$$W_s = \frac{1}{2} C V_{\max}^2$$

$$Q = \frac{\omega W_s}{P_d}$$

P_d = average dissipated power

$$P_d = \frac{1}{2} \omega C V_{\omega}^2 / Q$$

J. Number of Dynamic Cycles an Ion Experiences

The number of cycles of the dynamic potential that an ion sees is given by

$$n = \frac{L\omega}{2\pi v_z}$$

where

v_z = axial velocity

$$n = \frac{L\omega}{2\pi \left(\frac{2eV_z}{m} \right)^{1/2}}$$

III. Size and Weight

A. Double-Focused Spectrometer

The z -axis transmission determines the length of the magnet air gap. The smallest angle exist for the exit side of the magnetic analyzer.

$$l_g = 2z_m$$

$$l_i = l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m$$

$$= r_e \left[\theta_e + \frac{\left(-\frac{1}{G_e} - G_e + 2 \cos 2^{1/2} \theta_e \right)}{2^{1/2} \sin 2^{1/2} \theta_e} \right] + \left[\theta_m + \frac{\left(-\frac{1}{G_m} + \cos \theta_m \right)}{\sin \theta_m} \right] r_m$$

$$z_m = l_i \left(\frac{kT}{eV_m} \right)^{1/2}$$

$$= r_e \left[\theta_e + \frac{\left(-\frac{1}{G_e} - G_e + 2 \cos 2^{1/2} \theta_e \right)}{2^{1/2} \sin 2^{1/2} \theta_e} \right] \left(\frac{kT}{eV_m} \right)^{1/2} + r_m \left[\theta_m + \frac{\left(-\frac{1}{G_m} + \cos \theta_m \right)}{\sin \theta_m} \right] \left(\frac{kT}{eV_m} \right)^{1/2}$$

$$= r_m \left\{ \frac{\left(1 - \frac{1}{G_m} \right)}{(1 - G_e)} \left[\theta_e + \frac{\left(-\frac{1}{G_e} - G_e + \cos 2^{1/2} \theta_e \right)}{2^{1/2} \sin 2^{1/2} \theta_e} \right] + \theta_m + \frac{\left(-\frac{1}{G_m} + \cos \theta_m \right)}{\sin \theta_m} \right\} \left(\frac{kT}{eV_m} \right)^{1/2}$$

$$v_m = \left(\frac{2e}{m} V_m \right)^{1/2} = r_m B \frac{e}{m}$$

$$(V_m)^{1/2} = r_m B \left(\frac{e}{2m} \right)^{1/2}$$

$$z_m = \frac{\left(2kT \frac{m}{e^2} \right)^{1/2}}{B} \left\{ \theta_e + \frac{2^{1/2} (1 + \cos 2^{1/2} \theta_e)}{\sin 2^{1/2} \theta_e} + \theta_m + \frac{(1 + \cos \theta_m)}{\sin \theta_m} \right\}$$

where $G_e = G_m = -1$.

The symmetric cases are used since they provide the shortest ionic path lengths. The second order alpha correction can be made by curved entrance and exit boundaries at the magnetic sector.

$$l_g \simeq \frac{2(2)^{1/2} f_2}{e B_m} (kT m_h)^{1/2} (M_{\max})^{1/2} \left[\theta_e + \theta_M + \frac{2^{1/2} (1 + \cos 2^{1/2} \theta_e)}{\sin 2^{1/2} \theta_e} + \frac{(1 + \cos \theta_M)}{\sin \theta_M} \right]$$

Let

$$\Phi_e = \theta_e + \frac{2^{1/2} (1 + \cos 2^{1/2} \theta_e)}{\sin 2^{1/2} \theta_e}$$

$$\Phi_m = \theta_m + \frac{1 + \cos \theta_m}{\sin \theta_m}$$

$$\Phi_{me} = \Phi_e + \Phi_m$$

m_h = mass of the hydrogen atom

$$l_g = \frac{2(2)^{1/2} f_2}{e B_m} (kT m_h)^{1/2} (M_{\max})^{1/2} \Phi_{me}$$

The weight of the magnet is given by

$$W_m = d_m u_m$$

where

d_m = density of the magnet material

U_m = volume of the magnet

$$U_m = L_m [(r_m + X_s)^2 - (r_m - X_s)^2] \frac{\theta_M}{2}$$

$$= \frac{L_m}{2} \theta_M (4X_s) r_m$$

$$= 2L_m \theta_M X_s r_m$$

$$U_m = 2L_m (3\ell_g) \theta_M r_m$$

$$= 6 \frac{f_1}{f_2} \frac{B_m}{H_m} \ell_g^2 \theta_M r_m$$

$$= 6 \frac{f_1}{f_2} \frac{B_m}{H_m} \ell_g^2 \theta_M 2X_0 M_{\max}$$

$$= 12 \frac{f_1}{f_2} \frac{B_m}{H_m} \ell_g^2 \theta_M M_{\max} X_0$$

$$A_s = A_0 \left(\frac{e V_m}{kT} \right)^{1/2} \sin \alpha = \left(\frac{e V_m}{kT} \right)^{1/2} \sin \alpha X_0 \ell_0$$

$$= \frac{e r_m B_m \sin \alpha X_0 \ell_0}{2^{1/2} f_2 (kT m_h)^{1/2} (M_{\max})^{1/2}}$$

$$= \frac{e B_m \sin \alpha \ell_0 X_0 (2X_0 M_{\max})}{f_2 (kT m_h)^{1/2} (M_{\max})^{1/2} 2^{1/2}}$$

$$= 2^{1/2} \frac{e B_m \sin \alpha \ell_0 X_0^2 (M_{\max})^{1/2}}{f_2 (kT m_h)^{1/2}}$$

$$\ell_0 = 4Z_m = 2\ell_g$$

$$X_0 = \left(\frac{A_s f_2 (kT m_h)^{1/2}}{2^{1/2} e B_m \sin \alpha \ell_0 (M_{\max})^{1/2}} \right)^{1/2}$$

$$\ell_0 = \frac{4(2)^{1/2} (kT m_h)^{1/2} f_2 M_{\max}^{1/2} \Phi_{me}}{e B_m}$$

$$W_m = \theta_M d_m 12 \frac{f_1}{f_2} \frac{B_m}{H_m} M_{\max}$$

$$\times \left(\frac{A_s f_2 (kT m_h)^{1/2}}{2^{1/2} e B_m \sin \alpha 2\ell_g (M_{\max})^{1/2}} \right)^{1/2} \ell_g^2$$

$$= \theta_M d_m 6 \frac{f_1}{f_2} \frac{B_m}{H_m} M_{\max}^{3/4} \left(\frac{A_s f_2 (kT m_h)^{1/2}}{2^{1/2} e B_m \sin \alpha} \right)^{1/2} \ell_g^{3/2} 2^{1/2}$$

$$= 6 \theta_M d_m \frac{f_1}{f_2} 2^{1/2} \frac{B_m}{H_m} \left(\frac{A_s f_2 (kT m_h)^{1/2}}{e B_m \sin \alpha} \right)^{1/2}$$

$$\times M_{\max}^{3/4} 4 \left(\frac{f_2}{e B_m} \right)^{3/2} \Phi_{me}^{3/2} (kT m_h)^{3/4} M_{\max}^{3/4}$$

$$W_m = 24 \theta_M d_m f_2 f_1 \left(\frac{B_m}{H_m} \right)_{cgs} 2^{1/2} \left(\frac{A_s}{\sin \alpha} \right)^{1/2}$$

$$\times \frac{\Phi_{me}^{3/2}}{(e B_m)^2} kT m_h M_{\max}^{3/2}$$

If z-axis focusing is used, the following conditions are valid:

$$\ell_0 \neq 2\ell_g$$

The magnet weight becomes

$$(W_m)_f = 48 (2)^{3/4} d_m \frac{f_1}{f_2} \left(\frac{B_m}{H_m} \right)_{cgs}$$

$$\times \theta_m \frac{A_s^{1/2} f_2^{5/2} M_{\max}^{7/4} (m_h kT)^{5/4} \Phi_{me}^2}{(\sin \alpha)^{1/2} \ell_0^{1/2} B_m^{5/2} e^{5/2}}$$

$$\frac{(W_m)_f}{W_m} = \frac{2(2)^{1/4} \Phi_{me}^{1/2} f_2^{1/2} M_{\max}^{1/4} (m_h kT)^{1/4}}{\ell_0^{1/2} B_m^{1/2} e^{1/2}}$$

Let

$$\frac{\ell_0}{2\ell_g} = \delta$$

$$\frac{(W_m)_f}{W_m} = \frac{1}{\delta^{1/2}}$$

$$\frac{(r_m)_f}{r_m} = \frac{1}{\delta^{1/2}}$$

$$\frac{(X_0)_f}{X_0} = \frac{1}{\delta^{1/2}}$$

$$X_0 = \frac{1}{2^{3/4}} \left(\frac{A_s f_2}{e B_m \sin \alpha} \right)^{1/2} M_{\max}^{-1/4} (k T m_h)^{1/4} 2^{1/2} \left[\left(\frac{4 (2)^{1/2} f_2}{e B_m} \right) (k T m_h)^{1/2} (M_{\max})^{1/2} \Phi_{me} \right]^{1/2}$$

$$X_0 = \frac{2^{1/2}}{2^2} \left(\frac{A_s}{\sin \alpha} \right)^{1/2} \Phi_{me}^{-1/2} M_{\max}^{1/2}$$

$$r_m = 2 X_0 M_{\max}$$

$$r_m = \frac{1}{2^{1/2}} \left(\frac{A_s}{\sin \alpha} \right)^{1/2} \Phi_{me}^{-1/2} M_{\max}^{1/2}$$

$$\frac{l_g}{r_m} = \frac{4}{e B_m} \left(\frac{\sin \alpha k T m_h}{A_s} \right)^{1/2} f_2 \Phi_{me}^{3/2}$$

The half width of the electric plates z_e must be large enough to prevent ion capture; therefore,

$$\frac{\frac{l_0}{2} - z_e}{l_e} \geq \frac{\frac{l_0}{2} - z_m}{l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m}$$

$$z_e = \frac{l_0}{2} \left[1 - \frac{l_e}{l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m} \right]$$

$$+ \frac{z_m l_e}{l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m}$$

$$= \left[\frac{\frac{l_0}{2} (l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m) + z_m l_e}{l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m} \right]$$

$$l_0 = 4 z_m$$

$$z_e = z_m \frac{[2(l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m) + l_e]}{(l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m)}$$

$$= z_m \left[1 + \frac{l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m}{l_e + l_{ei} + r_e \theta_e + l_{im} + r_m \theta_m} \right]$$

$$z_e = z_m \left[1 + \frac{\frac{1}{2} \Phi_e + \Phi_m}{\Phi_{me}} \right]$$

$$z_e = \frac{2^{1/2} f_2}{e B_m} (k T m_h)^{1/2} (M_{\max})^{1/2} \left[\Phi_{me} + \frac{1}{2} \Phi_e + \Phi_m \right]$$

$$z_e = \frac{2^{1/2} f_2}{e B_m} (k T m_h)^{1/2} (M_{\max})^{1/2} \left[\frac{3}{2} \Phi_e + \Phi_m \right]$$

The radial extent of the electric sector Δr is given by

$$\Delta r = 2 X_s = \frac{1}{3} z_e$$

$$\Delta r = \frac{2^{1/2} f_2}{3 e B_m} (k T m_h)^{1/2} (M_{\max})^{1/2} \left[\frac{3}{2} \Phi_e + \Phi_m \right]$$

If z -axis focusing is used

$$z_e = 2 l_0$$

$$\Delta r = \frac{1}{3} l_0$$

The ion path length is given by

$$Y = Y_e + Y_m$$

$$= (\Phi_e + 2 \Phi_m) r_m$$

$$= \frac{1}{2^{1/2}} \left(\frac{A_s}{\sin \alpha} \right)^{1/2} M_{\max}^{1/2} \frac{(\Phi_e + 2 \Phi_m)}{(\Phi_{me})^{1/2}}$$

B. Quadrupole Spectrometer

For the quadrupole, the size and weight are influenced by the power consumption. Typically, instruments on a space flight mission are given a weight penalty that is related to the power consumption. For a given weight-to-power penalty, an optimized design can be made. It is for this reason that the power equations must be established before the weight can be computed.

$$P_d = \frac{1}{2} \frac{(4 \epsilon_0 L)}{Q} \omega V_\omega^2$$

$$= \frac{1}{2} \frac{4 \epsilon_0 L}{Q} \omega \frac{q^2 r_0^4 \omega^4}{(4)^2 e^2} m^2$$

$$= \frac{\epsilon_0 L q^2 r_0^4 \omega^5 m_h^2 M_{\max}^2}{8 Q e^2}$$

$$n = \frac{L \omega}{2 \pi \left(\frac{2e}{m} V_z \right)^{1/2}} \geq 3.5 M^{1/2}$$

with

$$\Delta m = 1$$

$$\omega \geq \frac{3.5(2\pi)}{L} \left(\frac{2eV_z}{m} \right)^{1/2}$$

$$P_d = \frac{\epsilon_0 L q^2 r_0^4 m_h^2 M_{\max}^2 (3.5)^5 (2\pi)^5 (2eV_z/m_h)^{5/2}}{8Q e^2 L^5}$$

$$= 2^4 2^{1/2} \frac{\epsilon_0}{Q} \left(\frac{e}{m_h} \right)^{1/2} q^2 \left(\frac{r_0}{L} \right)^4 (3.5)^2 V_z^{5/2} M_{\max}^2$$

From the expression for the limiting current density, the radius can be obtained.

$$A_0 = \pi r_0^2$$

$$A_s = \frac{A_0 e V_z \sin^2 \theta}{kT}$$

$$A_s = \frac{\pi r_0^2 e V_z \sin^2 \theta}{kT}$$

$$= \frac{\pi r_0^2 V_z e}{(2.7)^2 (2.5)^2 M_{\max}^2 kT}$$

$$= \frac{\pi q r_0^4 m_h M_{\max} \omega^2 e}{(2.7)^2 (2.5)^2 M_{\max}^2 4e kT}$$

$$= \frac{\pi q r_0^4 m_h \omega^2}{4 (2.7)^2 (2.5)^2 M_{\max} kT}$$

$$= \frac{\pi q r_0^4 m_h (3.5)^2 (2\pi)^2 2eV_z}{4 (2.7)^2 (2.5)^2 M_{\max} kT L^2 m_h}$$

$$= \frac{\pi e q r_0^4 (3.5)^2 \pi^2 V_z}{(2.7)^2 (2.5)^2 M_{\max} kT L^2}$$

where

$$\frac{m}{\Delta m} = M_{\max}$$

$$r_0^4 \geq \frac{(2.7)^2 (2.5)^2 M_{\max} kT L^2}{2q (3.5)^2 \pi^3 V_z} A_s$$

The power can be related to the length by

$$P_d = \left[\frac{2^4 2^{1/2} \epsilon_0}{L^4} \frac{\left(\frac{e}{m_h} \right)^{1/2} a}{Q} (3.5)^5 V_z^{5/2} M_{\max}^2 \right]$$

$$\times \left[\frac{(2.7)^2 (2.5)^2 M_{\max} kT L^2 A_s}{e (3.5)^2 \pi^3 q V_z} \right]$$

$$= \frac{2^4 2^{1/2} \epsilon_0}{(m_h e)^{1/2} Q} q V_z^{3/2} \frac{M_{\max}^3}{L^2} kT \frac{(2.7)^2 (2.5)^2}{\pi^3} A_s$$

The weight of the rods is given by

$$W_r = k_1 \pi r_q^2 L$$

where

r_q = radius of the rods

$$r_q = 1.15 r_0$$

The weight plus the weight penalty is given by

$$W = 4k_1 \pi L (1.32) r_0^2 + k_2 P_d$$

where

k_1 = density of the rod material

k_2 = weight to power penalty

$$W = 4k_1 \pi 1.32 \frac{(2.7) (2.5) M_{\max}^{1/2} (kT)^{1/2} A_s^{1/2}}{2^{1/2} q^{1/2} \pi^{3/2} V_z^{1/2} (3.5) e^{1/2}} L^2$$

$$+ \frac{k_2 2^4 \epsilon_0 q V_z^{3/2} M_{\max}^3 kT (2.7)^2 (2.5)^2}{(m_h e)^{1/2} Q \pi^3 L^2} A_s$$

$$W = \alpha_1 L^2 + \frac{\alpha_2}{L^2}$$

$$\frac{dW}{dL} = 2\alpha_1 L - 2\frac{\alpha_2}{L^3} = 0$$

$$L^4 = \frac{\alpha_2}{\alpha_1}$$

$$L = \left(\frac{\alpha_2}{\alpha_1} \right)^{1/4}$$

$$L = \frac{\left(\frac{k_2}{k_1}\right)^{1/4} \frac{2 \epsilon_0^{1/4}}{(m_h e)^{1/8}} \frac{q^{1/4} V_z^{3/8} M_{\max}^{3/4} (kT)^{1/4}}{Q^{1/4} \pi^{3/4}} \frac{(2.7)^{1/2} (2.5)^{1/2} A_s^{1/4}}{2^{1/2}}}{\frac{\pi^{1/4} (1.32)^{1/4} (2.7)^{1/4} (2.5)^{1/4} M_{\max}^{1/8} (kT)^{1/8}}{2^{1/8} q^{1/8} \pi^{3/8} V_z^{1/8} (3.5)^{1/4} e^{1/8}} A_s^{1/8}}$$

$$L = (3.5)^{1/4} \left(\frac{k_2}{k_1}\right)^{1/4} \frac{2^{5/8} \epsilon_0^{1/4} q^{3/8} V_z^{1/2} M_{\max}^{5/8} (kT)^{1/8}}{(m_h)^{1/8} Q^{1/4} \pi^{5/8} (1.32)^{1/4}} (2.7)^{1/4} (2.5)^{1/4} A_s^{1/8}$$

$$r_0 = \frac{(2.7)^{1/2} (2.5)^{1/2} M_{\max}^{1/4} (kT)^{1/4} A_s^{1/4}}{(e)^{1/4} q^{1/4} (3.5)^{1/2} \pi^{3/4} V_z^{1/4}} \times \frac{(3.5)^{1/8} (k_2/k_1)^{1/8} 2^{9/16} \epsilon_0^{1/8} q^{3/16} V_z^{1/4} M_{\max}^{5/16}}{2^{1/4} (m_h)^{1/16} Q^{1/8} \pi^{5/16} (1.32)^{1/8}} (2.7)^{1/8} (2.5)^{1/8} A_s^{1/8} (kT)^{1/16}$$

$$r_0 = \frac{(2.7)^{5/8} (2.5)^{5/8} (3.5)^{1/8} 2^{5/16} \epsilon_0^{1/8} A_s^{5/16} M_{\max}^{9/16} (k_2/k_1)^{1/8} (kT)^{5/16}}{(1.32)^{1/8} q^{1/16} Q^{1/8} \pi^{17/16} (m_h)^{1/16} e^{1/4}}$$

$$W_r = \pi k_1 (1.32) r_0^2 L = \frac{\pi k_1 (1.32) (2.7)^{5/4} (2.5)^{5/4} (3.5)^{1/4} 2^{9/8} \epsilon_0^{1/4} A_s^{5/8} M_{\max}^{9/8} (k_2/k_1)^{1/4} (kT)^{5/8}}{(1.32)^{1/4} q^{1/8} Q^{1/4} \pi^{17/8} (m_h)^{1/8} e^{1/2}}$$

$$\times \frac{(3.5)^{1/4} (k_2/k_1)^{1/4} \frac{2^{9/8}}{2^{1/2}} \epsilon_0^{1/4} q^{3/8} V_z^{1/2} M_{\max}^{5/8} (kT)^{1/8} (2.7)^{1/4} (2.5)^{1/4} A_s^{1/8}}{(1.32)^{1/4} (m_h)^{1/8} Q^{1/4} \pi^{9/8}}$$

$$W_r = \frac{(3.5)^{1/2} (1.32)^{1/2} (k_1 k_2)^{1/2} q^{1/4} (2.7)^{3/2} (2.5)^{3/2} \epsilon_0^{1/2} 2^{13/4} V_z^{1/2} M_{\max}^{7/4} (kT)^{3/4} A_s^{3/4}}{\pi^{14/8} (m_h)^{1/4} Q^{1/2}}$$

IV. Voltages

A. Double-Focused Spectrometer

$$V_m = \frac{B_m^2 r_m^2 e}{f_z^2 2m}$$

$$(V_m)_{\min} = \frac{B_m^2 r_m^2 e}{f_z^2 2m_h M_{\max}}$$

$$= \frac{B_m^2 e A_s}{2 f_z^2 m_h M_{\max} 4 \sin \alpha} \Phi_{me}^{-1} M_{\max}$$

$$(V_m)_{\min} = \frac{B_m^2 e A_s}{4 f_z^2 m_h \sin \alpha \Phi_{me}}$$

$$(V_m)_{\max} = \frac{B_m^2 e A_s M_{\max}}{4 f_z^2 m_h \sin \alpha \Phi_{me} M_{\min}}$$

$$(V_m)_{\max} = \frac{B_m^2 e A_s M_R}{4 f_z^2 m_h \sin \alpha \Phi_{me}}$$

where

$$M_R = \frac{M_{\max}}{M_{\min}}$$

The voltage on the electric sector plates is given by

$$V_e = 2 V_m \ln \frac{r_2}{r_1}$$

$$= 2 V_m \ln \frac{r_e + \frac{\Delta r}{2}}{r_e - \frac{\Delta r}{2}}$$

$$V_e = 2 V_m \ln \frac{1 + \frac{\Delta r}{2 r_e}}{1 - \frac{\Delta r}{2 r_e}} \simeq 2 V_m \frac{\Delta r}{r_e}$$

$$\frac{\Delta_r}{r_e} = \frac{\Delta r}{r_m} = \frac{2^{1/2} f_z (kT m_h)^{1/2} (M_{\max})^{1/2} [(3/2) \Phi_e + \Phi_m]}{3 e B_m} = \frac{2 f_z}{3 e B_m} \left(\frac{\sin \alpha kT m_h}{A_s} \right)^{1/2} \Phi_{me} [(3/2) \Phi_e + \Phi_m]$$

$$V_e = \frac{4 f_z}{3 e B_m} \left(\frac{\sin \alpha kT m_h}{A_s} \right)^{1/2} \Phi_{me} [(3/2) \Phi_e + \Phi_m] V_m$$

$$((V_m)_{\min})_f = \frac{(V_m)_{\min}}{\delta}$$

B. Quadrupole Spectrometer

$$V_\omega = \frac{q m r_0^2 \omega^2}{4e}$$

$$\omega = \frac{3.5 (2\pi) \left(\frac{2eV_z}{m_h} \right)^{1/2}}{L} = \frac{3.5 (2\pi) \left(\frac{2eV_z}{m_h} \right)^{1/2} 2^{1/2}}{(3.5)^{1/4} (k_2/k_1)^{1/4} 2^{9/8} \frac{\epsilon_0^{1/4} q^{3/8} V_z^{1/2} M_{\max}^{5/8} (kT)^{1/8}}{(m_h)^{1/8} Q^{1/4} \pi^{5/8} (1.32)^{1/4}} (2.7)^{1/4} (2.5)^{1/4} A_s^{1/8}}$$

$$\omega = \frac{(3.5)^{3/4} (2\pi) (\pi)^{5/8} (1.32)^{1/4} Q^{1/4} (2e)^{1/2} (k_1/k_2)^{1/4}}{(2.7)^{1/4} (2.5)^{1/4} 2^{13/8} q^{3/8} (kT)^{1/8} A_s^{1/8} \epsilon_0^{1/4} M_{\max}^{5/8} m_h^{3/8}}$$

$$V_\omega = \frac{q m_h M_{\max} (3.5)^{3/2} (2\pi)^2 \pi^{5/4} (1.32)^{1/2} Q^{1/2} 2e 2 (k_1/k_2)^{1/2}}{4e (2.7)^{1/2} (2.5)^{1/2} 2^{9/4} q^{3/4} (kT)^{1/4} A_s^{1/4} \epsilon_0^{1/2} M_{\max}^{5/4} m_h^{3/4}} \times \frac{(2.7)^{5/4} (2.5)^{5/4} (3.5)^{1/4} 2^{9/8} \epsilon_0^{1/4} A_s^{5/8} M_{\max}^{9/8} (k_2/k_1)^{1/4} \frac{(kT)^{5/8}}{2^{1/2}}}{(1.32)^{1/4} q^{1/8} Q^{1/4} \pi^{17/8} m_h^{1/8} e^{1/2}}$$

$$V_\omega = \frac{2^{3/8} q^{1/8} (3.5)^{7/4} (2.7)^{3/4} (2.5)^{3/4} (2\pi)^2 Q^{1/4} (kT)^{3/8} m_h^{1/8} A_s^{1/2} M_{\max}^{7/8} (k_1/k_2)^{1/4}}{4 e^{1/2} \pi^{7/8}}$$

V. Power

A. Double-Focused Spectrometer

The power that is consumed by the analyzer supply is given by

$$P_a = \frac{V_m}{R_m}$$

where R_m is the resistance of the divider string that is across the analyzer supply.

The R_m can be very large; however, the scan rate would be limited by the resistance and the capacitance of the electrodes.

$$(P_a R_m)_{\max} = V_m^2 = \frac{B_m^4 e^2 A_s^2 \pi M_R^2}{64 f_z^2 m_h^2 \sin^2 \alpha \Phi_{me}^2}$$

$$((P_a R_m)_{\max})_f = \frac{(P_a R_m)_{\max}}{\delta^2}$$

B. Quadrupole Spectrometer

$$P_d = \frac{W_r}{k_2}$$

$$P_d = \frac{(3.5)^{1/2} (1.32)^{1/2} (k_1/k_2)^{1/2} q^{1/4} (2.7)^{3/2} (2.5)^{3/2} \epsilon_0^{1/2} 2^{13/4} V_z^{1/2} (kT)^{3/4} A_s^{3/4} M_{\max}^{7/4}}{\pi^{7/4} m_h^{1/4} Q^{1/2}}$$

VI. Required Voltage Stability

A. Double-Focused Spectrometer

$$V_m = \frac{B^2 r_m^2 e}{2m}$$

$$\frac{\Delta V}{V} = \frac{2\Delta B}{B} - \frac{\Delta m}{m}$$

$$\frac{\Delta m}{m} = \frac{2\Delta B}{B} - \frac{\Delta V}{V}$$

These variations produce a shift in the mass calibration; however, the resolutions would not suffer unless they are produced by a high-frequency noise source.

If the voltage on the electric sector does not follow the scan voltage, the velocity focusing would suffer. This would result in a resolution reduction.

The displacement at the object slit which would be produced by a lack of tracking in the electric sector is given by

$$X_{mc} = -2\beta_e r_e + 2\beta_m r_m$$

Let

$$\beta_e = \beta_m + \Delta\beta$$

$$\begin{aligned} X_{mc} &= 2\Delta\beta r_e + 2\beta_m (r_m - r_e) \\ &= 2\Delta\beta r_e \end{aligned}$$

if

$$r_m = r_e$$

$$\Delta\beta = \frac{1}{2} \Delta V_e / V_e$$

$$\begin{aligned} \frac{\Delta V_e}{V_e} &= \frac{X_{mc}}{r_e} \\ &= \frac{X_0}{2r_m} \end{aligned}$$

$$= \frac{1}{4M_{\max}} \left(\begin{array}{l} \text{symmetric electric} \\ \text{and magnetic sectors} \end{array} \right)$$

$$\frac{\Delta V_e}{V_e} = \frac{1}{4M_{\max}} \left(2 - \frac{r_m}{r_e} \right)^2 \left(\begin{array}{l} \text{symmetric electric} \\ \text{sector and a } 90^\circ \\ \text{magnetic sector} \end{array} \right)$$

B. Quadrupole Spectrometer

$$\frac{m}{\Delta m} = \frac{0.75}{1 - \frac{\gamma}{\gamma_{\max}}}$$

where γ is the ratio of the static to the dynamic potentials

$$\gamma_{\max} - \gamma = \Delta\gamma = 7.5\gamma_{\max} \frac{\Delta m}{m}$$

$$\frac{\delta(\Delta\gamma)}{\gamma_{\max}} = \frac{0.75 \delta(\Delta m)}{m}$$

$$\begin{aligned} \frac{\delta\gamma}{\gamma_{\max}} &= \frac{0.75 \delta(\Delta m)}{\frac{m}{\Delta m} \Delta m} \\ &= \frac{0.75 \delta(\Delta m)}{M_{\max} \Delta m} \end{aligned}$$

Let

$$\frac{\delta(\Delta m)}{\Delta m} \leq 0.1$$

$$\frac{\delta\gamma}{\gamma_{\max}} \leq \frac{0.075}{M_{\max}}$$

$$V_\omega = \frac{q_m r_0^2 \omega^2}{4e}$$

$$\frac{\Delta V_\omega}{V_\omega} = \frac{\Delta m}{m}$$

$$\frac{\Delta V_\omega}{V_\omega} = \frac{1}{M_{\max}}$$

This variation effects the stability of the mass calibration; however, if the variation is caused by high-frequency noise the resolution would suffer.

The frequency variation is given by

$$\begin{aligned}\frac{\Delta\omega}{\omega} &= \frac{1}{2} \frac{\Delta m}{m} \\ &= \frac{1}{2} \frac{1}{M_{\max}}\end{aligned}$$

Low-frequency drifts would produce a shift in the mass calibration, but a high-frequency modulation would reduce the resolution.

The frequency variation should be less than

$$\frac{\Delta\omega}{\omega} \leq \frac{1}{Q} = 10^{-2}$$

so that the power consumption does not become excessive. Even when the frequency is highly stabilized the center frequency of the resonant secondary circuit must be stable, even though the rod voltage is regulated, because the dissipated power would become excessive.

$$\frac{P^*}{P_0} = [1 + Q^2 (\Delta\omega_0/\omega_0)^2]$$

where

ω_0 = center frequency

P_0 = dissipated power at the center frequency

VII. Mechanical Tolerance

A. Double-Focused Spectrometer

The electric sector has the most severe tolerance requirements, in comparison to the other components of the double focused instrument.

$$V_e = 2V_m \frac{\Delta r}{r_e}$$

$$\frac{\delta V_e}{V_e} = \frac{\delta(\Delta r)}{\Delta r}$$

$$\frac{\delta V_e}{V_e} = \frac{1}{4M_{\max}}$$

$$\begin{aligned}\frac{\delta(\Delta r)}{\Delta r} &= \frac{1}{4M_{\max}} \quad \left(\begin{array}{l} \text{symmetric electric} \\ \text{and magnetic sectors} \end{array} \right) \\ &= \frac{\left(2 - \frac{r_m}{r_e}\right)^2}{4M_{\max}} \quad \left(\begin{array}{l} \text{Symmetric electric} \\ \text{and } 90^\circ \text{ magnetic sectors} \end{array} \right)\end{aligned}$$

B. Quadrupole Spectrometer

$$r_0^2 = \frac{4eV_\omega}{qm\omega^2}$$

$$\frac{\Delta r_0}{r_0} = \frac{1}{2} \frac{\Delta m}{m}$$

$$= \frac{1}{2M_{\max}}$$

This is the tolerance for the rods. The tolerance for the spacing is given by

$$\begin{aligned}\frac{\Delta d}{d} &= \frac{2\Delta r_0}{4r_0} \\ &= \frac{1}{4M_{\max}}\end{aligned}$$

d = center line distance between two rods

VIII. Space Charge

A. Double-Focused Spectrometer

The effects of space charge occur over the entire ion path; however, the greatest effect is at the collector slit. As the ions converge to the collector slit the mutual repulsion produces a divergence force. Instead of the formation of a crossover at the collector slit, a waist would be formed. The dimension of the waist will be calculated.

$$\nabla \cdot E_x = \rho/\epsilon_0$$

where ρ is the space charge density.

The space charge density is assumed to be constant over the dimension x until the edge of the beam is reached. The space charge is assumed to be infinite in the y and z directions for the purpose of integration of the Poisson equation

$$E_x = \frac{\rho x}{\epsilon_0}$$

$$I = A \rho v_m$$

$$A = (2x)(2z_m)$$

$$\rho = \frac{I}{4xz_mv_m}$$

$$E_x = \frac{I}{4z_mv_m\epsilon_0}$$

$$\frac{mdv_x}{dt} = eE_x$$

$$\frac{v_m dv_x}{dy} = \frac{e}{m} E_x$$

$$= \frac{eI}{4mz_m\epsilon_0 v_m}$$

$$v_x = \frac{eIy}{4mz_m\epsilon_0 v_m^2} - \alpha v_m$$

$$\frac{v_m dx}{dy} = \frac{eIy}{4mz_m\epsilon_0 v_m^2} - \alpha v_m$$

$$\frac{dx}{dy} = \frac{eIy}{4mz_m\epsilon_0 V_m^3} - \alpha$$

$$X_{mc} = \frac{eIy^2}{8z_m\epsilon_0 v^3 m}$$

$$y = \frac{1}{2} r_m \theta_m + l_{mc}$$

$$\simeq r_m \left(\frac{\theta_m}{2} + \frac{\cos \theta_m - G_m}{\sin \theta_m} \right)$$

$$X_{mc} = \frac{x_0}{2}$$

$$= \frac{r_m}{4M_{\max}}$$

$$I = \frac{r_m 8 (m_h/e) M_{\max} z_m \epsilon_0 B^3 r_m^3 (e/m_h)^3}{4M_{\max} e M_{\max}^3 r_m^2 \left(\frac{\theta_m}{2} + \frac{\cos \theta_m - G_m}{\sin \theta_m} \right)^2}$$

$$I = \frac{2r_m^2 B_m^3 z_m \epsilon_0 e^2}{f_z^3 m_h^2 \left(\frac{\theta_m}{2} + \frac{\cos \theta_m - G_m}{\sin \theta_m} \right)^2 M_{\max}^3}$$

$$r_m^2 z_m = \left[\frac{1}{2^{1/2}} \left(\frac{A_s}{\sin \alpha} \right)^{1/2} \Phi_{me}^{-1/2} M_{\max}^{1/2} \right]^2 \\ \times \left[\frac{2^{1/2} f_z (kTm_h)^{1/2} M_{\max}^{1/2} \Phi_{me}}{e B_m} \right] \\ = \frac{f_z \left(\frac{A_s}{\sin \alpha} \right) M_{\max}^{3/2} (kTm_h)^{1/2}}{2^{1/2} B_m e}$$

$$I = \frac{2^{1/2} B_m^2 (kT)^{1/2} e \epsilon_0 A_s}{f_z^2 m_h^{3/2} M_{\max}^{3/2} \sin \alpha \left[\frac{\theta_m}{2} + \frac{1 + \cos \theta_m}{\sin \theta_m} \right]^2}$$

B. Quadrupole Spectrometer

The space charge in the quadrupole analyzer is assumed to be constant through the region of the quadrupole field

$$\nabla^2 V = \frac{\rho}{\epsilon_0}$$

$$\frac{\partial^2 V}{\partial X^2} + \frac{\partial^2 V}{\partial y^2} = \rho/\epsilon_0$$

$$V = \frac{(V_0 + V_c) y^2 - (V_0 - V_c) x^2}{r_0^2}$$

where

$$V_c = \frac{\rho r_0^2}{4\epsilon_0}$$

$$I = v_z \rho \pi r_0^2$$

$$v_z = \left(\frac{2e}{m} V_z \right)^{1/2}$$

$$V_c = \frac{i}{\pi \left(\frac{2e}{m} V_z \right)^{1/2} 4\epsilon_0}$$

This potential adds to the static potential on one pair of rods, while it subtracts from the static potential on the other rod pair. For this reason the effect of the space charge potential is considered to be a change in the ratio γ .

$$\gamma^* = \frac{V_D - V_c}{V_\omega} = \frac{V_D}{V_\omega} - \frac{V_c}{V_\omega} = \gamma_0 - \delta\gamma$$

$$\delta\gamma = \frac{\frac{I}{4\epsilon_0\pi \left(\frac{2eV_z}{m}\right)^{1/2}}}{\frac{qmr_0^2\omega^2}{4e}}$$

$$= \frac{I(e/m)^{1/2}}{\epsilon_0\pi q 2^{1/2} (V_z)^{1/2} \omega^2 r_0^2}$$

$$\delta\gamma \leq \frac{.075 \gamma_{\max}}{M_{\max}}$$

$$I \leq \frac{\epsilon_0\pi q (V_z)^{1/2} \omega^2 r_0^2 (0.075) \gamma_{\max}}{2^{1/2} \left(\frac{e}{m}\right)^{1/2} M_{\max}}$$

$$I = \frac{\epsilon_0\pi q (V_z)^{1/2} \omega^2 r_0^2 (0.075) \gamma_{\max}}{2^{1/2} \left(\frac{e}{m_h}\right)^{1/2} (M_{\max})^{1/2}}$$

$$I = \frac{\epsilon_0\pi q (V_z)^{1/2} (0.075) \gamma_{\max} (3.5)^{3/2} (2\pi)^2 \pi^{5/4} (1.32)^{1/2} Q^{1/2} (2e) (k_1/k_2)^{1/2}}{2^{1/2} \left(\frac{e}{m_h}\right)^{1/2} M_{\max}^{1/2} (2.7)^{1/2} (2.5)^{1/2} 2^{9/4} q^{3/4} (kT)^{1/4} A_s^{1/4} \epsilon_0^{1/4} M_{\max}^{5/8} m_h^{3/4}}$$

$$\times \frac{(2.7)^{5/4} (2.5)^{5/4} (3.5)^{1/4} 2^{9/8} \epsilon_0^{1/4} A_s^{5/8} M_{\max}^{9/8} (k_2/k_1)^{1/4} (kT)^{5/8}}{(1.32)^{1/4} q^{1/8} Q^{1/4} \pi^{17/8} m_h^{1/8} e^{1/2}}$$

$$I = \left(\frac{\epsilon_0\pi^{17/8} q^{1/8} 2^{29/8} (2.7)^{3/4} (2.5)^{3/4} (3.5)^{7/4} Q^{1/4} (0.075) \gamma_{\max} (V_z)^{1/2} (1.32)^{1/4}}{m_h^{5/8}} \right) \times ((kT)^{3/8} A_s^{3/8} (k_1/k_2)^{1/4})$$

$$I_{\max} = 2.56 \times 10^{-8} \text{ A}$$

IX. Conclusions

When the quadrupole mass spectrometer is compared with a double-focused mass spectrometer and both instruments are used with equivalent ion sources, which have a voltage spread of 10V, the quadrupole has about twice the weight and maximum power. The sizes of the two types are about the same. The maximum dynamic voltage for the quadrupole mass spectrometer is less than the static voltage for the double-focused mass spectrometer. The maximum ion current for the quadrupole is about four times that of the double-focused instrument; however, the ion source suffers before the ion current limit is reached for either instrument.

The voltage stability and mechanical tolerance are about the same for both instruments. With weight and power the bases for a comparison, the double-focused instrument seems to be the better.

A comparison of the quadrupole with the double-focused mass spectrometer is presented in Table 1. In this table, the weight of the double-focused instrument is the magnet weight only while the weight of the quadrupole is the weight of the four rods, only. The weight of the vacuum envelope for the double-focused instrument should be considerably less than that of the quadrupole, since it is

Table 1. Comparison of spectrometers

	Double focused						Quadrupole						Units	
	$M_{\max}$						$M_{\max}$							
Parameter	1	10	100	200	1000		1	10	100	200	1000			
Weight	0.001	0.037	1.1	3.2	3.5		0.001	0.058	2.9	9.5	160		lb	
Power	$1.44^{\odot} \times 10^{-3}$	$1.44^{\odot} \times 10^{-1}$	$1.44^{\odot} \times 10$	$5.76^{\odot} \times 10$	$1.44^{\odot} \times 10^3$	$^{\odot}$ Mass range; $R_m = 10^7$ ohms	0.0024	0.116	5.8	19.6	320		W	
Length	0.427	1.34	4.28	6.6	13.8	$3.5 r_m$	0.334	1.4	5.7	8.9	24		in.	
Width	0.244	0.77	2.44	3.46	7.2	$2 r_m$	0.156	0.56	2.06	3.03	7.26	$2r_0(1 + 2 \times 1.15)$	in.	
Thickness	0.215	0.675	2.15	3.09	6.7	$L_m + L_g$	0.156	0.56	2.06	3.03	7.26	$2r_0(1 + 2 \times 1.15)$	in.	
Voltage	$1.2^{\odot} \times 10^3$	$1.2^{\odot} \times 10^3$	$1.2^{\odot} \times 10^4$	$2.4^{\odot} \times 10^4$	$1.2^{\odot} \times 10^5$	$^{\odot}$ Mass range	8.7	63	460	830	3300		V	
Frequency	—	—	—	—	—		18	4.2	1	0.65	0.24		MHz	
Maximum ion current	2.66×10^{-6}	2.43×10^{-7}	7.66×10^{-9}	2.72×10^{-9}	2.43×10^{-10}		2.6×10^{-8}							A
Voltage stability	2.5×10^{-1}	2.5×10^{-2}	2.5×10^{-3}	1.2×10^{-3}	2.5×10^{-4}		0.08	8×10^{-3}	8×10^{-4}	4×10^{-4}	8×10^{-5}		$\Delta V/V$	
Mechanical tolerance	2.5×10^{-1}	2.5×10^{-2}	2.5×10^{-3}	1.2×10^{-3}	2.5×10^{-4}		2.5×10^{-1}	2.5×10^{-2}	2.5×10^{-3}	1.2×10^{-3}	2.5×10^{-4}		$\Delta d/d$	

much smaller; however, the combined weight of the magnet yoke, and the vacuum housing may be about equal to the weight of the quadrupole housing.

There are some techniques that can be used to reduce the weight that is presented in Table 1 for both of the instruments. For the double-focused instrument, z -axis focusing can be used which would allow a longer object slit. With an object slit four times as long, the weight of the magnet could be reduced by a factor of two. The maximum voltage would be reduced by a factor of 4, while the power would be reduced by a factor of 16. The minimum voltage would be reduced by a factor of 4 so that it would become 30 V. To further reduce the maximum voltage and power for a large mass range, two different radii can be used. This can be accomplished by using two collectors or by using a smaller angle of rotation and radius of curvature for the lighter masses, so that they are focused to the same collector. In the latter case, a suppressor potential would be applied to the beams so that they could be gated with a radius reduction by a factor of 4 and the power by a factor of 16. The resolution of the ion beam that has the smaller radius would be less, but for the lighter masses a smaller resolution would be adequate.

For the quadrupole instrument, the weight of the rods could be reduced by removing material from the center of the rods. The maximum ID of the rods would be determined by the required mechanical stability, in particular the stiffness required for the grinding process. It is

expected that the weight of the rods could be reduced by 25 percent by the removal of material at the center of the rod. It may be possible to construct the rods of some lighter material, such as metalized ceramic.

For the analysis of the quadrupole instrument, a particular mission was used. That mission had a weight-to-power penalty of $\frac{1}{2}$ lb/W. To minimize the effective weight, the actual weight was made to be equal to the weight penalty. For different missions the weight penalty may be different so that a difference design would be required to obtain the minimum effective weight.

The double-focused instrument requires the maximum power at the minimum mass number; therefore, with the primary emphasis on the maximum mass number, the maximum power consumption is a function of mass range and not the maximum mass number. For this reason, a weight-to-power penalty was not used for the design; however, if the mass range is large it should be used.

The symmetrical double-focused instrument has the least weight and the largest ion current; therefore, the design that is presented in Table 1 is based on a symmetrical electric and magnetic sectors. The angle of both sectors was taken to be 90° , since this angle provides the shortest, or very nearly the shortest, ion path length; however, a reduction in the magnet weight by a factor of two could be obtained by using a smaller angle for the magnetic sector with an increase in the ion path length.