# The Analyzer

- The analyzer is where the beam of ions generated in the ion source is separated into multiple beams each representing a single charge to mass ratio (ideally).
- We will deal mainly with magnetic sector instruments here although we will talk briefly about other separation methods later.
- Remember from our discussion of ion sources that our ion beam is a roughly rectangular shaped beam that is diverging in the y–direction (beam coordinates).
- Divergence or convergence in the z-direction need not concern us for the moment.

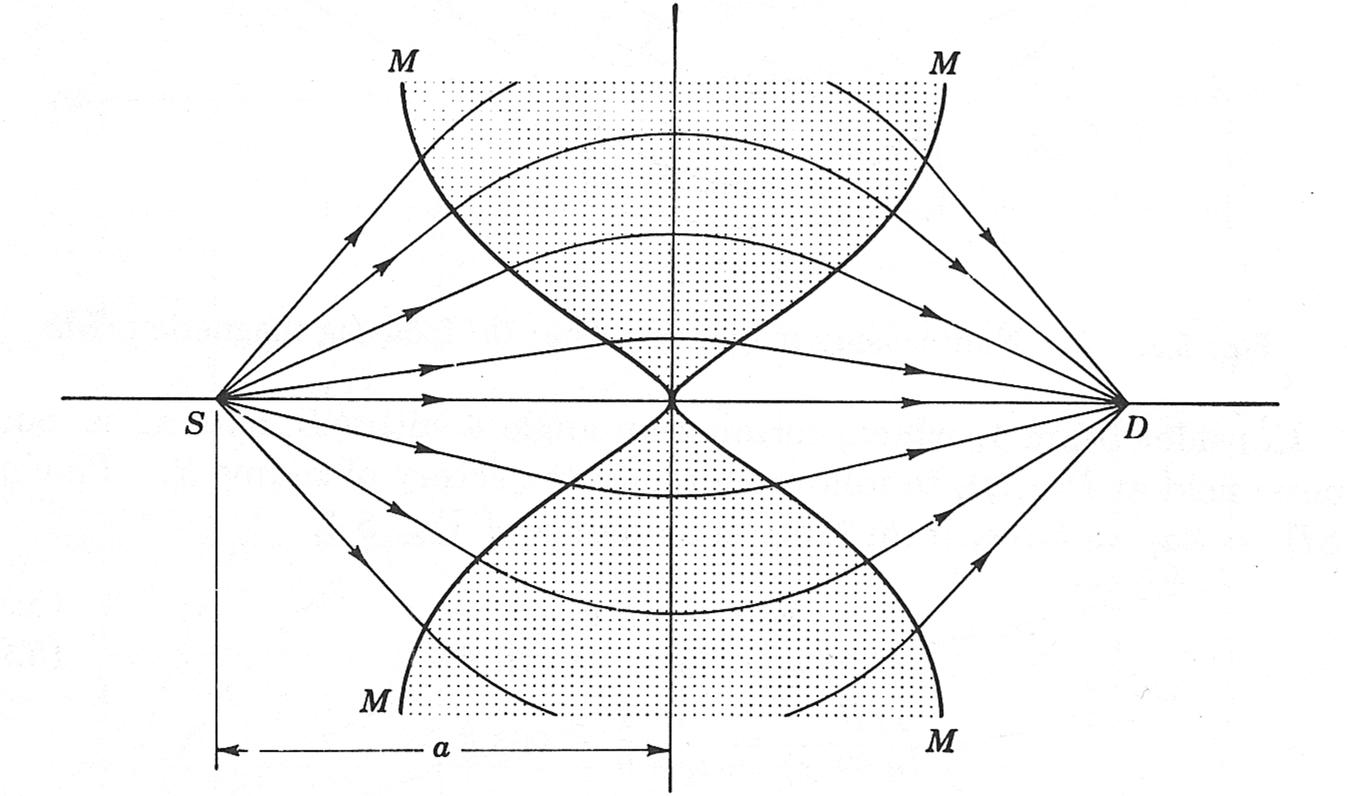
- An ion beam that continually diverged would result in poor separation of mass.

- Fortunately, however, most magnetic and electric shapes have some focusing properties (just as most random pieces of glass will focus some light).

- Just as in the case with light some shapes are better than others.

- By shaping the magnetic field (I will deal mainly with magnetic separation for the moment) properly it is possible to refocus the separated ion beams and thus maximize the mass separation.

- Is there an ideal shape?
- Sort of!
- The shape shown below will focus a highly divergent ion beam to a perfect focus.



# However, there are some restrictions:

- It only works for mono-energetic ions with the same m/q ratio. Variations in energy will cause blurring of the focal point and different m/q values will follow different paths.
- It assumes the ion source is a point. If the ion source has some dimension in the y-direction (again in beam coordinates) the focal point will not longer be a point (it will be both larger and blurrier).
- It assumes a perfect magnet, that is, the magnetic field starts and stops abruptly at the pole faces and has a value of zero outside the magnet and a constant value inside the pole faces.

# Real Magnets

- In light of the previous restrictions and the fact that the ideal shape is not easy to machine, real magnetic sector mass spectrometers are a compromise.

- They usually are an approximation to some segment of the ideal shape

- This means that the focusing is never perfect, the ion beam focuses to a fuzzy image of the exit slit

Factors that affect the size , or fuzziness, of the image:

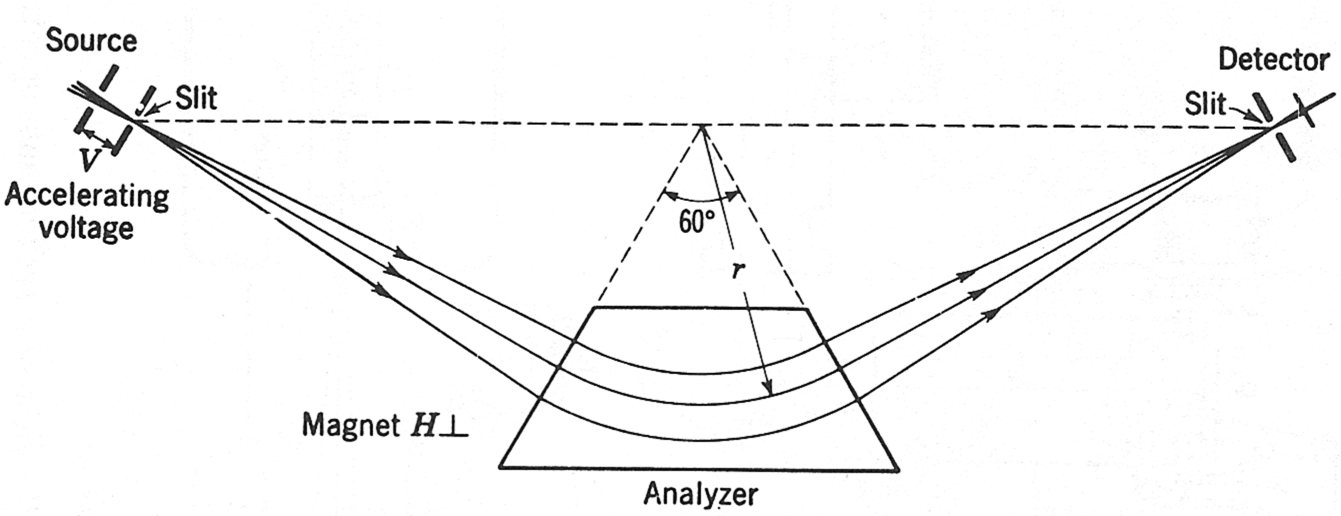
- Size of the source exit slit
- Divergence angle
- Magnet geometry
- Miscellaneous effects

# Nier Geometry

- The Nier Geometry has been the “workhorse” of magnetic sector mass spectrometry for many years

Characteristics:

- Magnet poles are sectors of a circle (the traditional sectors have been 60° and 90°)
- The ion beam nominally enters and exits the magnet at 90°
- Assuming an ideal magnet, the object focus (the exit slit of the source) and the image focus lie on a horizontal line that passes thru the apex of the magnet



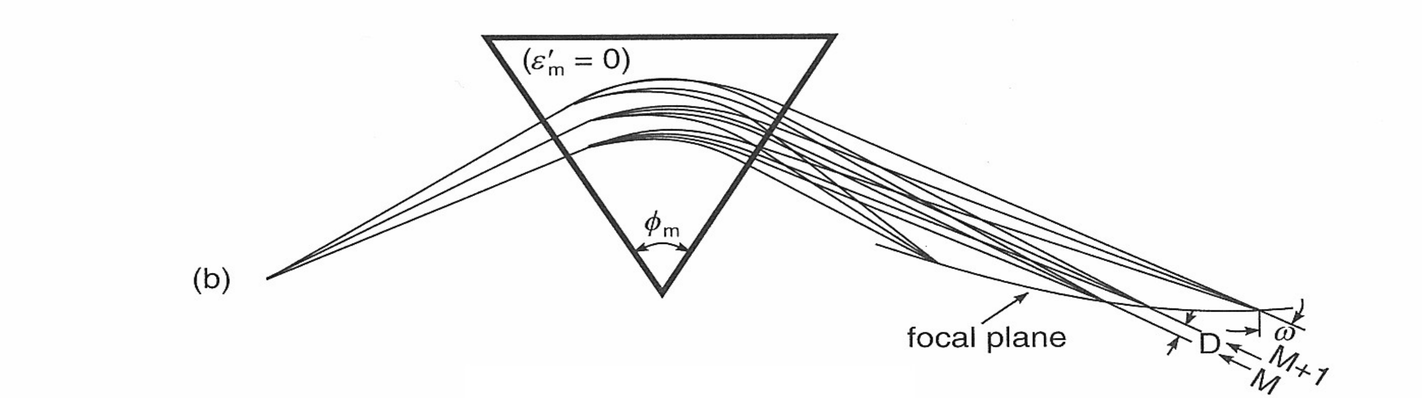
# Consequences of Nier Geometry

- Object and image focal points lie a distance D from the magnet given by:

$$D = \frac{R}{\tan\frac{\theta}{2}}$$

Where R is the radius of curvature, and θ is the sector angle. So for θ = $90^o$ R= D

- The Nier geometry achieves first order focusing
- Other masses come to focus on a curved focal plane that passes through the axial focal point



# Nier Geometry continued

- Advantages of Nier Geometry
  - Simple to machine and set up
  - Very compact footprint especially at $90^0$
  - Other sources of aberration can usually be ignored

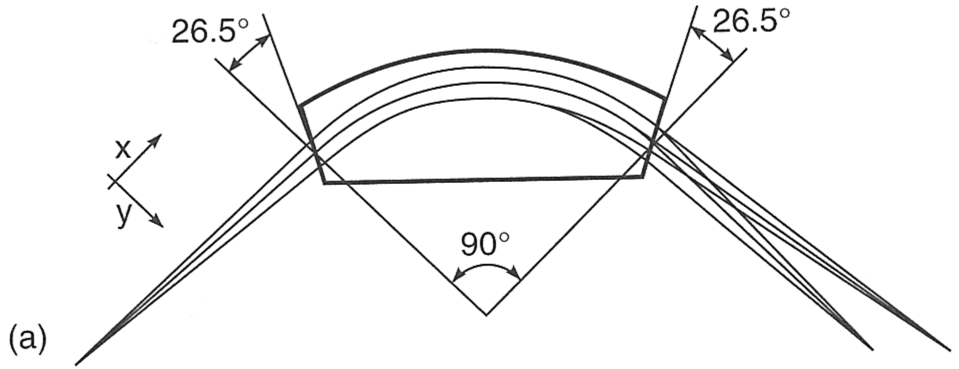
- Disadvantages
  - Focal plane curved, hard to set-up multiple detectors
  - Mass separation poor at high masses especially for small magnets
  - First order focusing limits resolution (typical beam width at focal point is 50% larger than width at source exit slit

To get around some of these problems we can go to what is known as extended geometry

# Extended Geometry

- By rotating the entrance and exit pole faces of the magnet so that the entrance and exit angles are no longer $90^0$ we can improve things:

- The focal plane becomes flat (or near flat) over a wide mass range
- The effective radius of curvature increases becoming twice the true radius at an angle of $26.5^o$
- This doubles the separation between masses and doubles the distance of the focal points from the magnet
- Most importantly we achieve second order focusing, the beam width increasing by about 15%



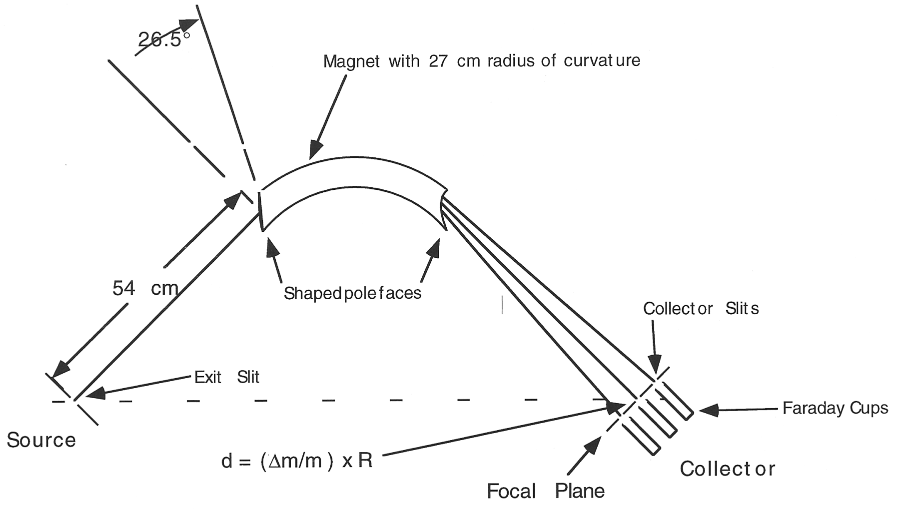
- Advantages of Extended geometry:
  1. Focal plane is relatively flat, multiple detectors easier to use
  2. Twice the mass separation for the same size Nier magnet
  3. Second order focusing improves mass resolution

- Disadvantages:
  1. Footprint larger
  2. Focal plane at an angle to the incoming beams, detectors must be staggered “en echelon”
  3. Other aberrations must be considered

- Disadvantage 2 can be gotten around, that is the focal plane can be made to intersect the beams at a right angle (for the axial beam)

# Extended Geometry as practiced by GV and precursors

- By shaping the pole faces and making the exit face angle adjustable it is possible to bring the focal plane at right angles to the axial beam:

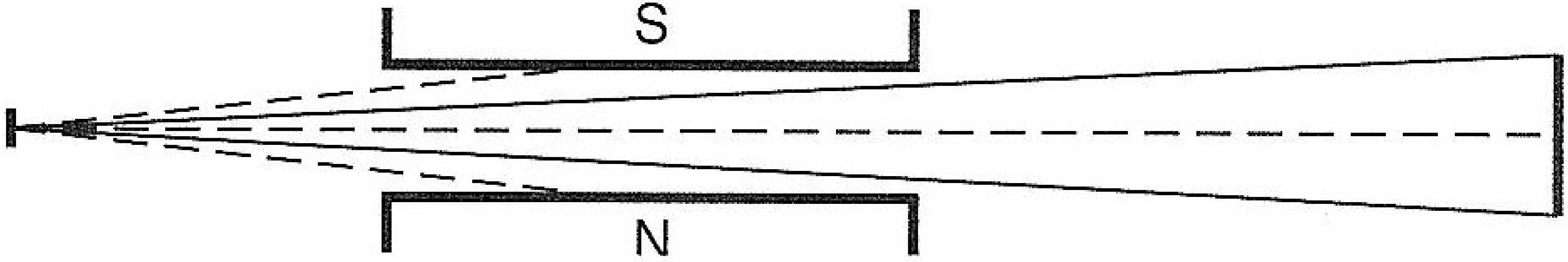


Effective radius of curvature is 2 x 27 = 54 cm. (R)

Figure 1: Highly Schematic drawing of a mass spectrometer with extended geometry and flat focal plane normal to the axial beam.

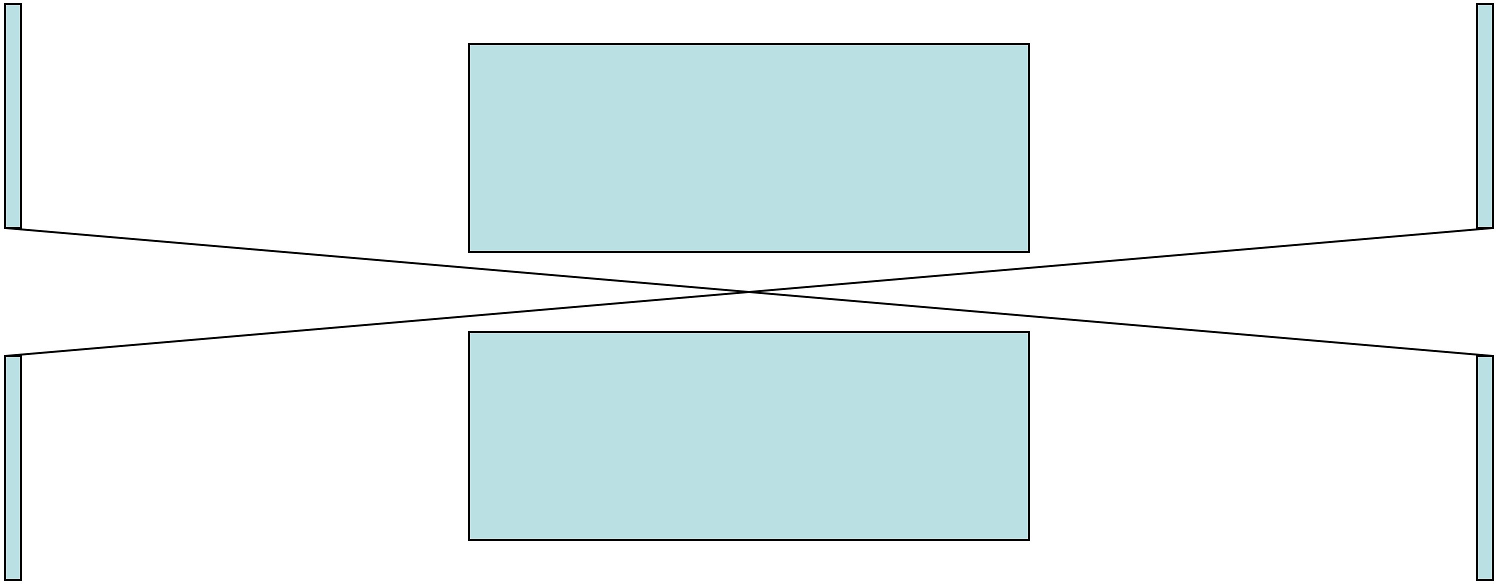
# The Z-direction and Fringe Fields

- If there is no z-focusing in the ion lens the ions diverge in the z-direction
- The flight tube internal dimension at the magnet pole gap determines the beam's z dimension and divergence



# Z-focusing

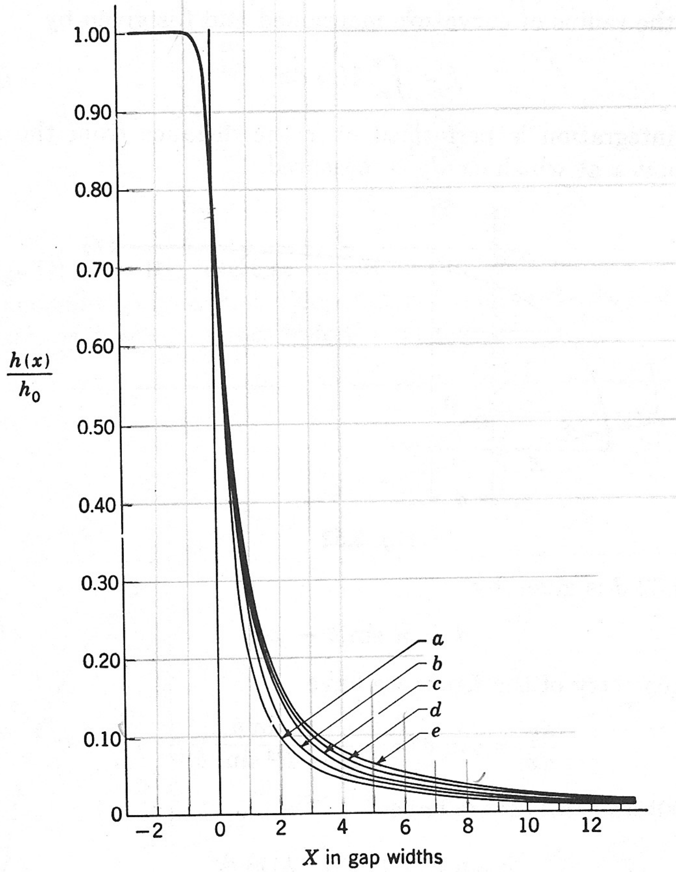
- With Z-focusing lenses we can confine the beam to the pole gap

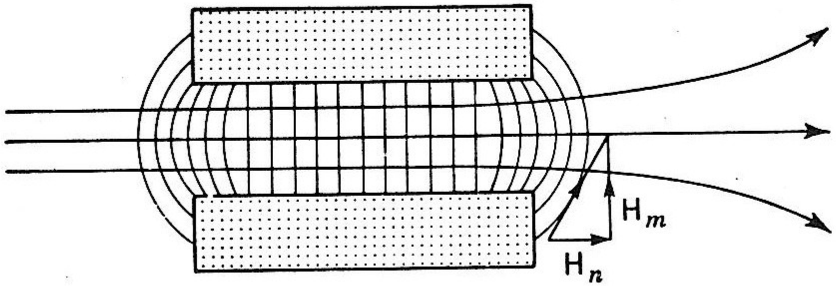


- However, Z-focusing is complicated by fringe fields and other factors

# Fringe Fields

- The magnetic field of the magnet extends outside of the pole face:





Characteristics of fringe field:

Strongly curved outside of magnet and just inside pole face

Lower field just inside pole face

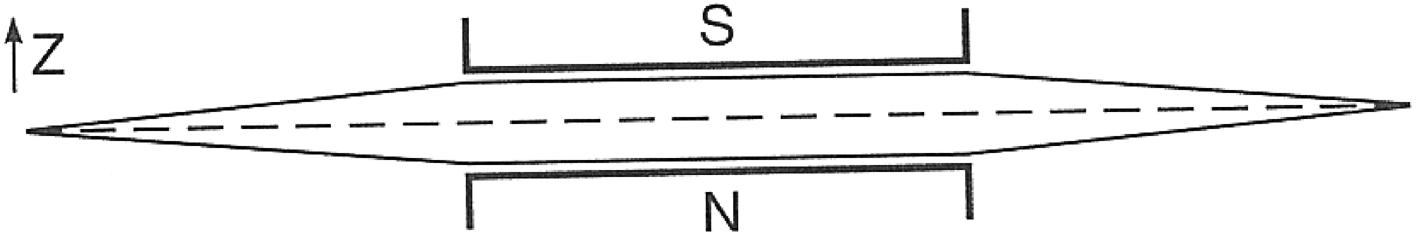
Strength depends on magnetic properties

Of magnet material and pole gap

# Effects of Fringe field

- In Nier magnet the fringe field moves the focal points and adds aberrations from a z component to the magnetic force
  - These aberrations can be mitigated somewhat by z-focusing

- In extended geometry the fringe field can be used to focus in the z-direction especially when combined with z-focusing lenses



- Still produces small amount of aberration

# Dispersion

- Dispersion is the actual physical distance between the focal points of two adjacent masses at the focal plane.

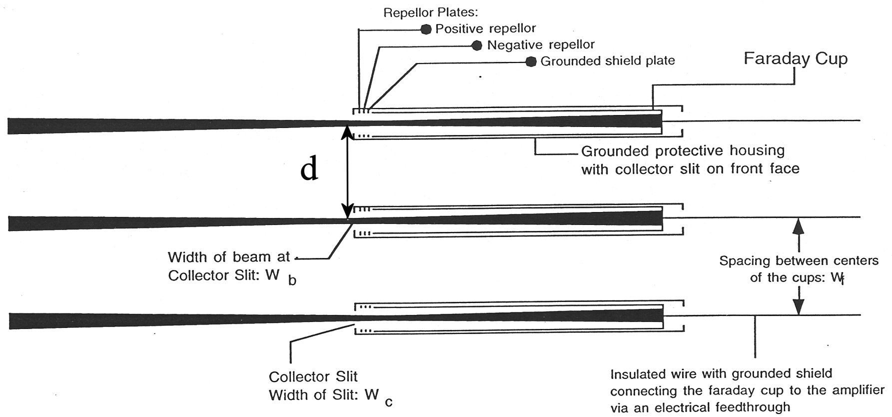


Figure 2: Diagram of three faraday cup collectors set for Sr spacing ($Sr^{87}$ in the axial position) for a mass spectrometer with an effective radius of 54 cm. Scale: 4x. Ion beams are diverging with half-angles of $1^{o}$

- Where d is the dispersion.

# Dispersion continued

- For a symmetrical mass spectrometer (i.e., where object and image distances are the same) there is a relatively simple equation to calculate dispersion:

$$d = \frac{\Delta m}{m} R_{eff}$$

- where $R_{eff}$ is the effective radius of curvature of the magnet (for a Nier magnet this is the actual radius of curvature, for extended geometry it is twice the real radius), m is the axial mass and $\Delta m$ is the difference in mass.
- Note this equation is a simplification of a more complex equation and is not exact for a number of reasons but is very close as long as $\Delta m$ is not too large.

# Dispersion

- For example, an extended geometry magnet with an $R_{eff}$ of 540 mm has a dispersion at mass 88 of 6.136 mm per amu but only 2.269 mm per amu at mass 238. These would be one half these numbers for a Nier magnet.

- Dispersion is also sometimes given as ppm of the effective radius, i.e.:

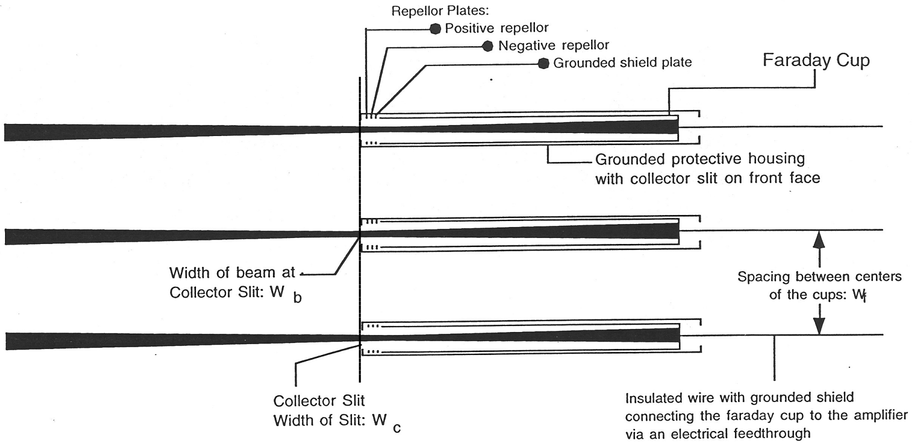
$$\frac{d}{R_{eff}} = \frac{\Delta m}{m} 1x10^6$$

- For the examples above:
- At mass 88 the dispersion is 11363 ppm.
- At mass 238 the dispersion is 4202 ppm.

- Note that the dispersion is independent of the magnet angle and ion energy.

- This equation can also be used for calculating any physical distance at the focal plane or converting a distance to mass equivalent. We will see more of this when we discuss resolution.

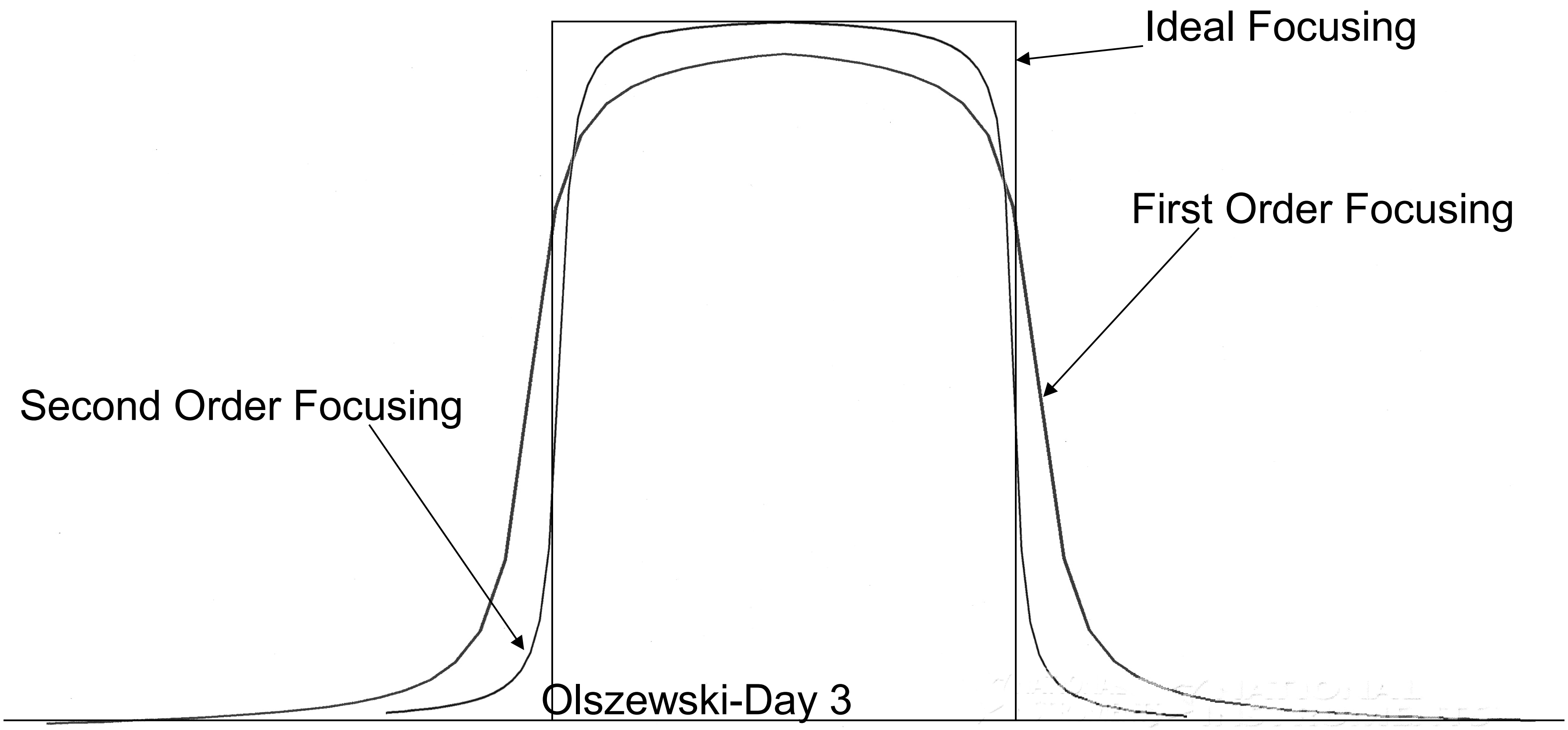
# At the focal plane



- Beams are isolated at focal plane by slits
- Slits must be wider than beam width at focal plane to allow total beam to reach detector and also to allow for variations in magnetic field and ion energy (Flat Topped Peaks)
- The ability to resolve two closely spaced peaks depends on the dispersion, the beam width at the focal plane and the collector slit width

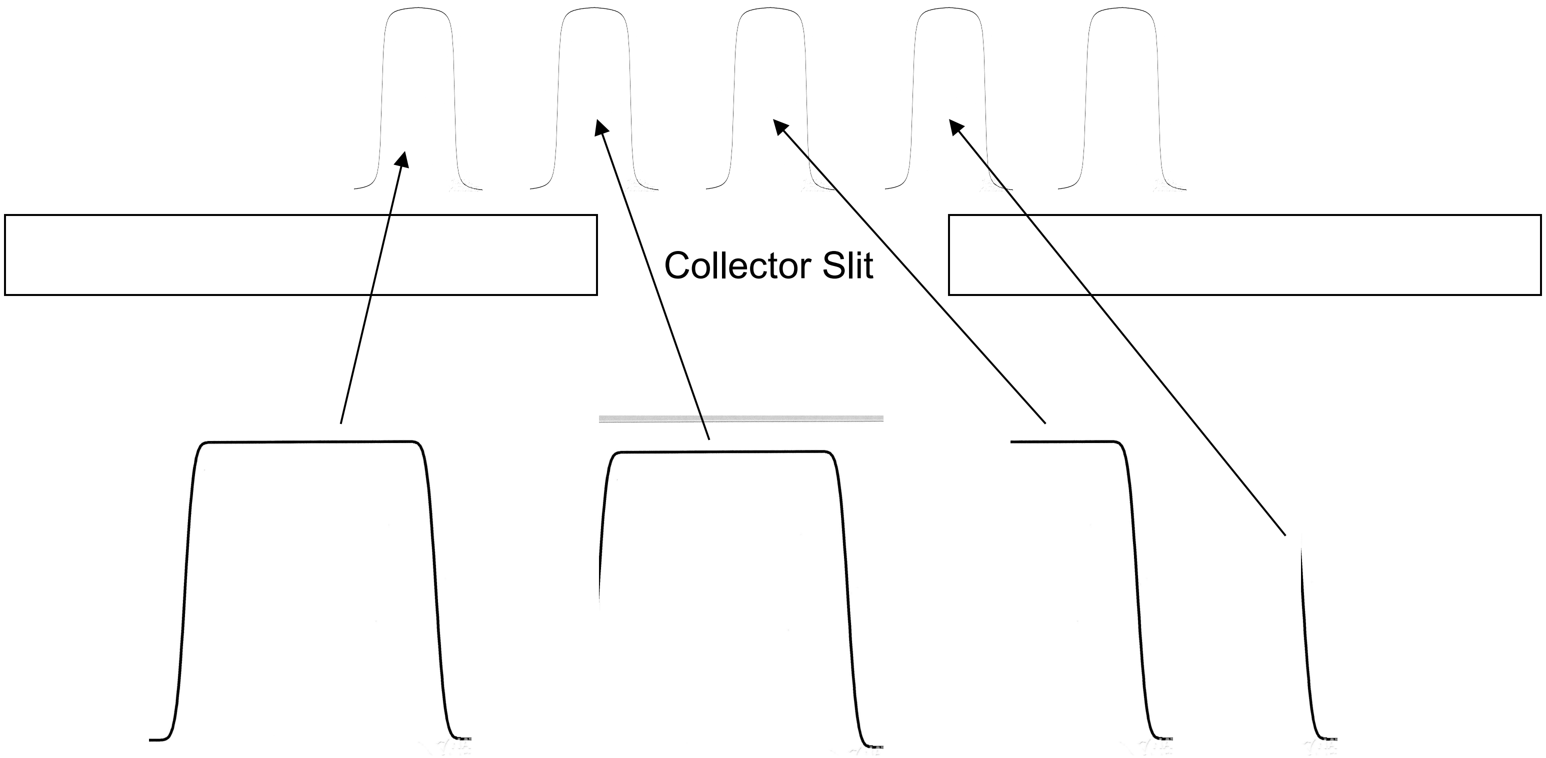
# Cross Section of Beam Intensity at the Focal Plane

- These are cross sections through the beam at the focal plane along the medial plane

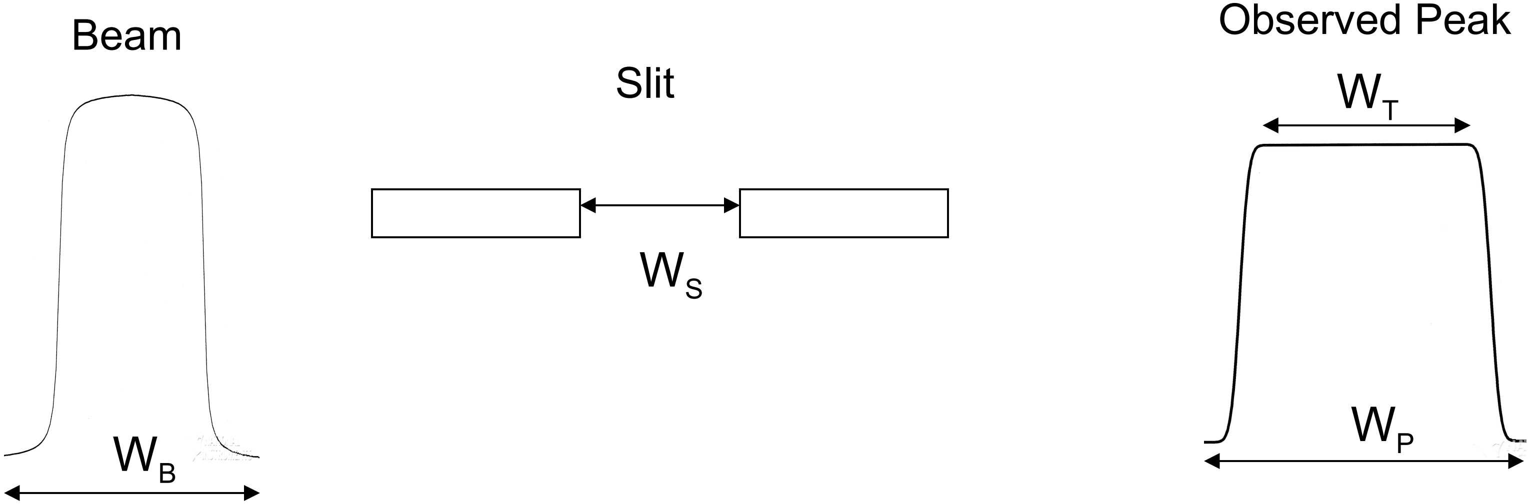


# What do we see at the detector?

- Observed peak is wider than beam
- Peak top is flat (intensity does not change) while beam is in slit
- Intensity of Peak is the beam integrated over its whole width



# Calculating beam parameters



$$W_T = W_S - W_B$$

$$W_p = W_S + W_B$$

# Some Examples

- For $W_B$ = 0.35 mm and $W_S$ = 1.0 mm
  - $W_T$ = 0.65 mm and $W_P$ = 1.35 mm
- Note that these values are mass independent

- However, in terms of amu these values will vary depending on the mass we are looking at:
  - At mass 88
    - $W_B$ = 0.057 amu, $W_S$ = 0.163 amu, $W_T$ = 0.106 amu and $W_P$ = 0.220 amu
  - At mass 208
    - $W_B$ = 0.135 amu, $W_S$ = 0.385 amu, $W_T$ = 0.250 amu and $W_P$ = 0.520 amu

- $W_P$ represents the minimum spacing between two peak before they overlap at the baseline level, $W_P$ / 2 represents the spacing at which two peaks overlap at peak top center

- We can now look at mass spectrometer resolution

# Resolution

- Resolution is a measure of the ability to distinguish two closely spaced ion beams.
- Resolution is usually defined as:

$$R = \frac{m}{\Delta m_{10\%}}$$

where R is the resolution, m is the mass whose resolution is being measured and $\Delta m_{10\%}$ is the mass change necessary to get the peak intensity down to 10% of its maximum intensity.

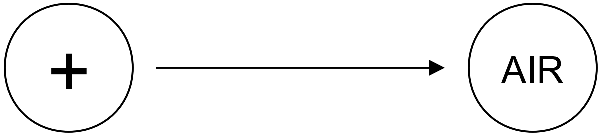
# Resolution continued

- The mass at 10% intensity can be hard to calculate, it is sometimes more useful to use the baseline width calculated above:
  - For Sr: 88/0.11 = 800
  - For Pb: 208/0.260 = 800
- Notice that this is also the radius of curvature (effective) divided by one-half the peak width ($W_P$)
- So for example at mass 208 we could have two peaks separated by 0.260 amu and still measure the correct beam intensity (just barely) if we centered on the peak top of each peak
- However, in mass spectrometers with multiple detectors the limiting factor is usually how close we can get the detectors to one another.

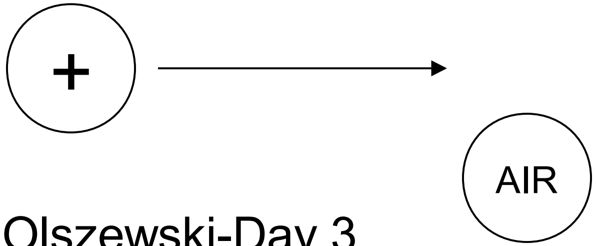
# Abundance Sensitivity

- Even with perfect focusing we would find a widening of the beam width at the focal plane, especially on the low mass side of the beam
- This is because of interactions between the ion beam and residual air in the mass spectrometer
- We can distinguish two end member types of interaction (with most interactions falling in between):

Head-On Collision:



Glancing Collision:



# Head-On Collisions

- Direction of motion of ion changed little, some energy is lost by the ion however
- If this occurs after the ion has passed through the magnet, No Problem
- If it occurs before or during passage through the magnet the path of the ion will be different from the ions of the same mass that have not lost energy.
- The effect is greatest when the energy loss is high or if the loss occurs early in the flight path.
- Energy loss causes the ion to behave like a slightly less massive ion, so it will reach the focal plane at a mass position slightly lower than its true mass
- This produces a tail on the low mass side of an ion beam which for intense ion beams can be significant evens a few amu away.
- This makes it difficult to measure a very small beam on the low mass side of a very intense beam
- For example:

  $^{234}$U next to $^{235}$U, $^{236}$U and $^{237}$U next to $^{238}$U

  $^{230}$Th next to $^{232}$Th

# Glancing Collisions

- Ion loses little energy but its direction of travel can change significantly
- The effect is greatest if it occurs early in the flight path
- Changes in direction are symmetric
- The result is to produce tails on both the high and low mass sides of the beam, or alternatively to widen the base of the beam

## Abundance Sensitivity

- Abundance sensitivity is a measure of the extent of this effect and is defined as:

$$A = \frac{I_{M-1}}{I_M} \cdot 10^6$$

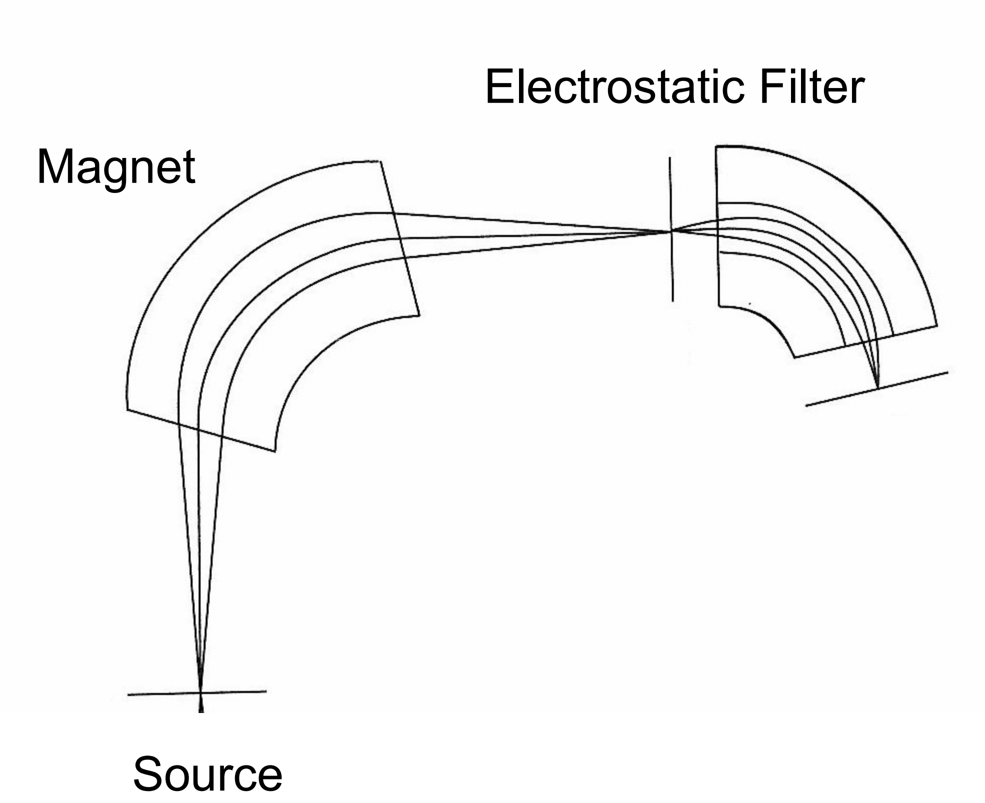
Where A = abundance sensitivity in ppm, $I_{M-1}$ is the intensity 1 amu below the main peak at mass M and $I_M$ is the intensity of the main peak

# Abundance Sensitivity

- Depends on the quality of the vacuum in the mass spectrometer
- For machines like the Sector 54, Isolab or Triton with only a magnetic sector at a pressure of $10^{-9}$ torr the typical abundance sensitivities are 1 to 10 ppm
- This means that isotope ratios lower than a few times $10^{-5}$ would be difficult to measure
- It is difficult to get vacuums much below $10^{-9}$ torr with machines this size (and for other reasons)
- So how can we improve abundance sensitivity?

# Improving Abundance Sensitivity

- In lieu of a perfect vacuum there are ways to improve abundance sensitivity
- Add an electrostatic filter:

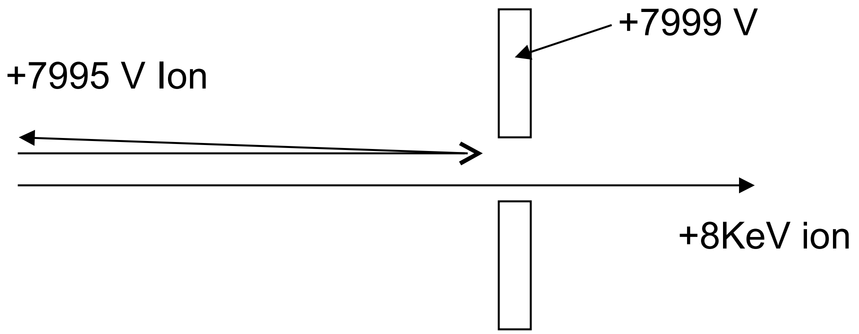


Works reasonably well, usually gives a factor of 10 or so improvement in Abundance sensitivity

Disadvantages:
- Bends beam
- Still lets through range of energies
- Does little to remove glancing collision particles

# Improving Abundance Sensitivity continued

- WARP, RPQ filters
- Both use an aperture to pass only ions that have lost less than a certain amount of energy:



- A quadrupole or long aperture is used to remove ions entering at high angle (the glancing collisions)