SPECTROMETERS

1st Lecture: 24/01/2023, 12:00 - 13:00

Definitions; Formalism; Main ion-optical elements

2nd Lecture: 25/01/2023, 10:30 - 11:30

Higher Orders ; Exemples

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Literature

• Optics of Charged Particles, Hermann Wollnik, Academic Press, Orlando, 1987.

• The Optics of Charged Particle Beams, David.C Carey, Harwood Academic Publishers, New York 1987.

• A First- and Second-Order Matrix Theory for the Design of Beam Transport Systems and Charged Particle Spectrometers. Karl L. Brown. SLAC Report-75. June 1982
https://cds.cern.ch/record/283218/files/SLAC-75.pdf

Computing Codes:

• COSY INFINITY 10.0 Beam Physics Manual
https://www.bmtdynamics.org/cosy/manual/COSYBeamMan100.pdf

• GICOSY Manual https://web-docs.gsi.de/~weick/gicosy/

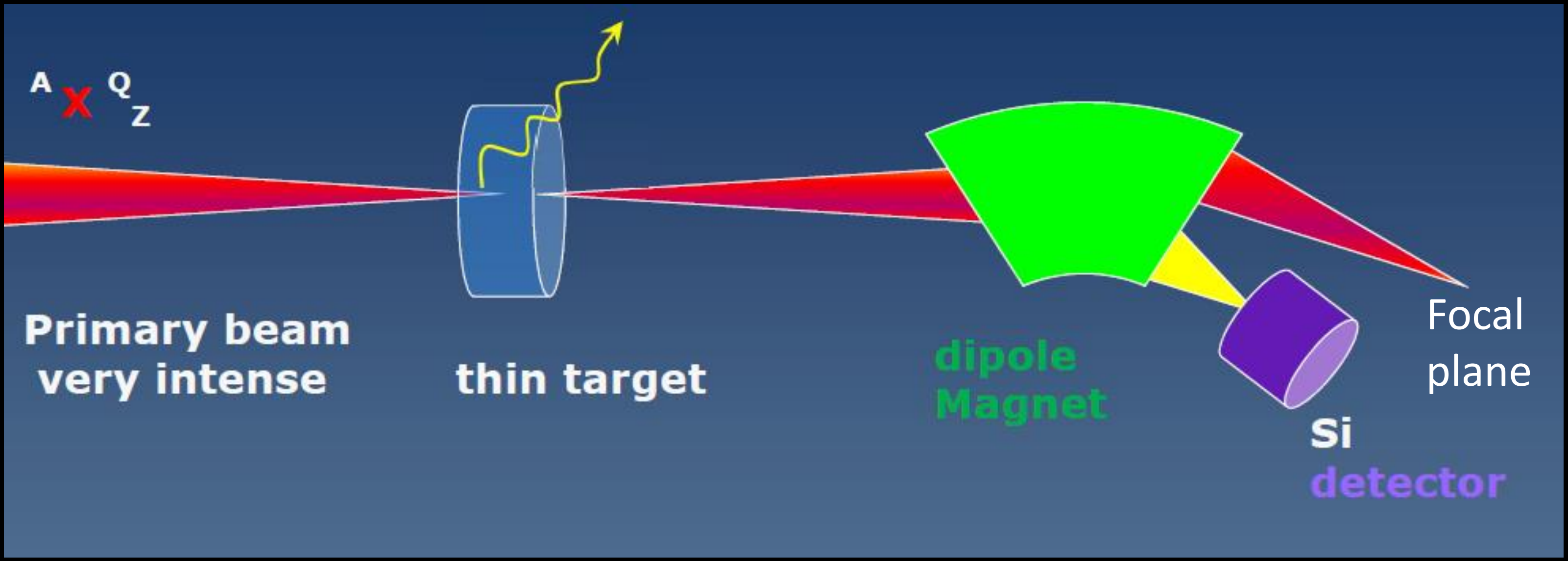
• TRANSPORT http://aea.web.psi.ch/Urs_Rohrer/MyWeb/trans.htm

Thanks B. Jacquot and Franck Varenne/ GANIL for some material used in this course

What is a Spectrometer?

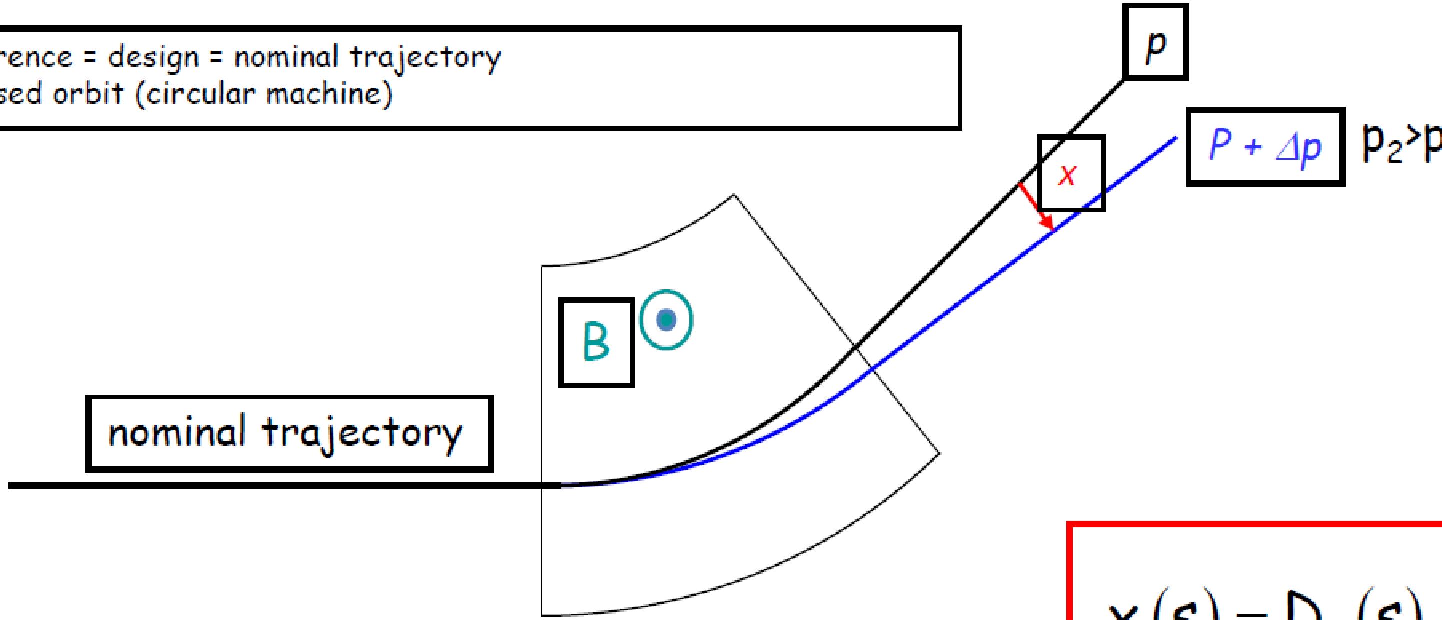
In the broadest sense a spectrometer is any instrument that is used to measure the variation of a physical characteristic over a given range.

A dipole magnet is the simplest electromagnetic spectrometer to scan on mass-to-charge ratio (m/q)

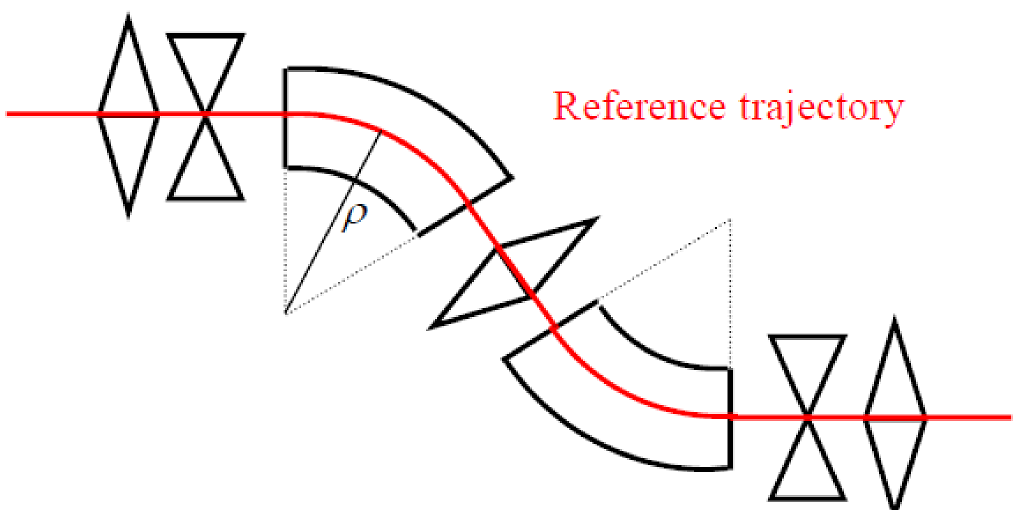


Dispersion

reference = design = nominal trajectory
= closed orbit (circular machine)



$$x(s) = D_x(s)\,\frac{\Delta p}{p}$$

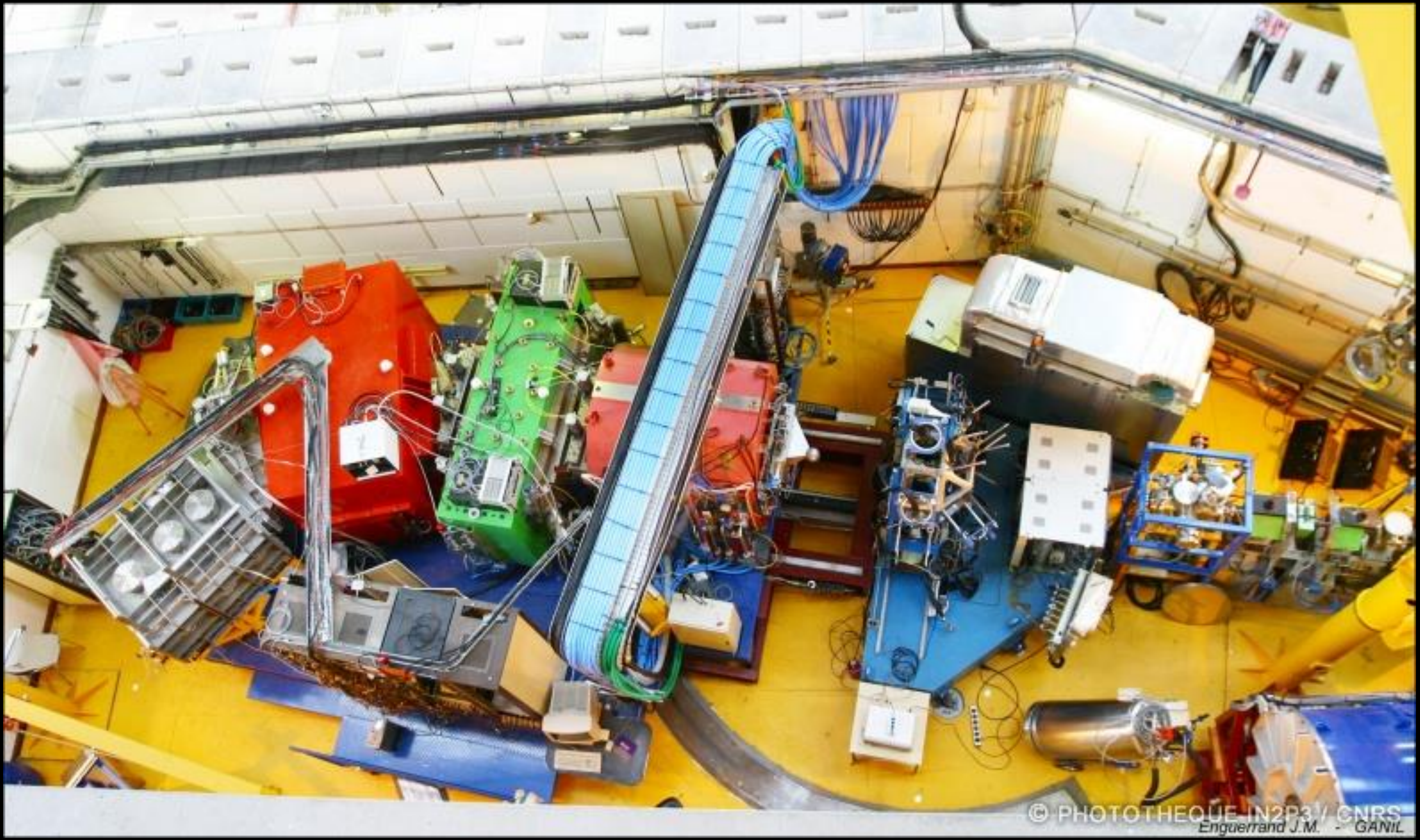


GSI FRS Germany

BIGRIPS RIKEN Japan

LISE (wien filter)
GANIL, France

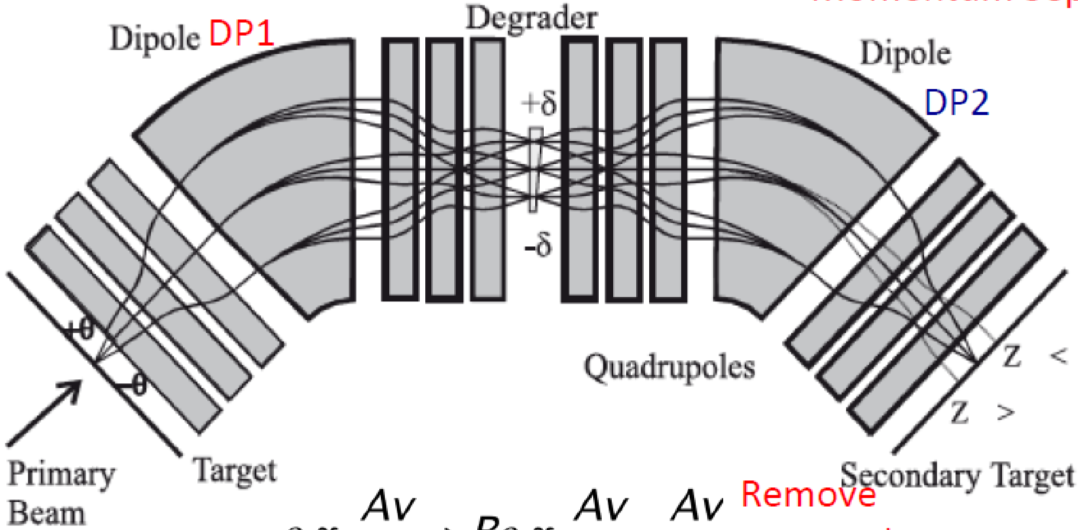
VAMOS
GANIL, France

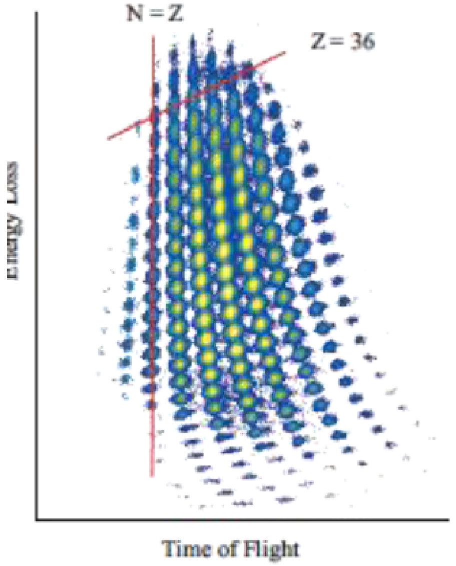


Fragment Separator - FRS

A/Z separation

Momentum Separation





DP1 $\rho \propto \frac{Av}{QB} \Rightarrow B\rho \propto \frac{Av}{Q} = \frac{Av}{Z}$

Remove primary beam $10^{12} \rightarrow 10^{8}$

Degrader $\propto \frac{AZ^2}{E}$

Degrader + DP2 $\propto \frac{A^3}{Z^2}$

Reduction $10^{8} \rightarrow 10^{6}$

$$v_2^2 = v_1^2 - d\,\frac{Z^2}{Z+N}$$

$$v_2 = v_1 \frac{(B\rho)_2}{(B\rho)_1}$$

Energy loss $\mu\ Z^2$

T_{vol} (Target - detector)= $\frac{d}{v} \propto \frac{A}{Z}$

Why it works?

Thanks to the Lorentz force F and Newton's second law

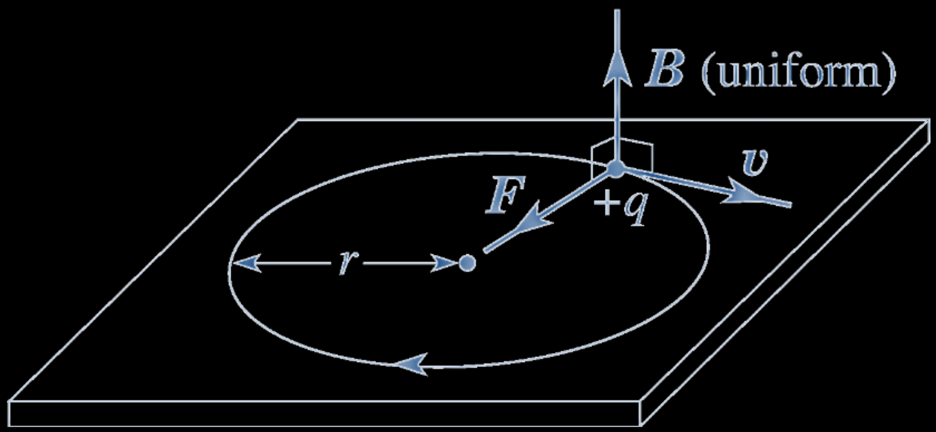
1. Lorentz force: A charged particle moving in an electromagnetic field experiences a force.

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$$

Electic Force **Magnetic Force**

This force causes a centripetal acceleration and consequently a circular motion of the particle in the medium based on the equations described below.

2. **Newton's second law**

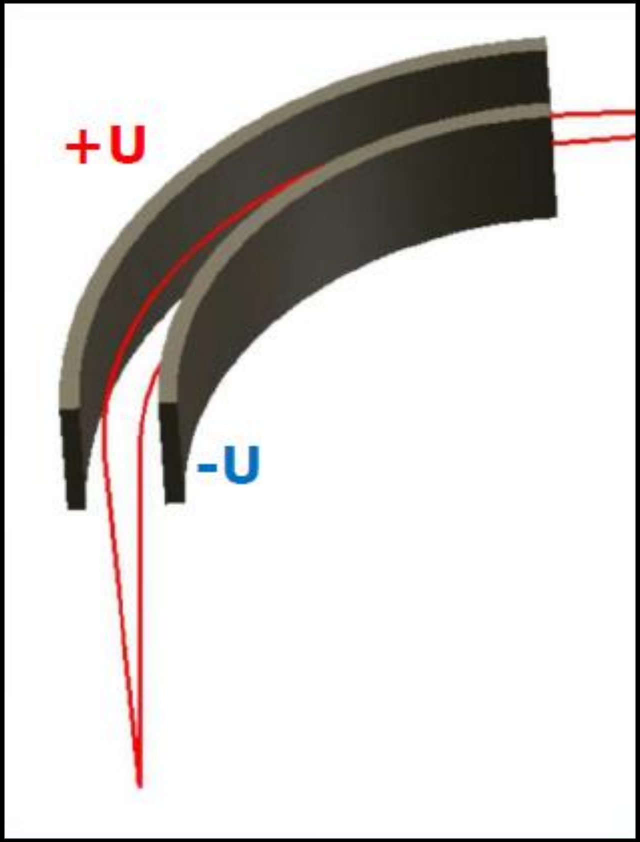


$$\boldsymbol{F} = m\,\boldsymbol{a}$$

$$F_{centripetal} = \frac{mv^2}{r}$$

Radius r → ρ

Electrostatic selection :



$$F = q\,E$$

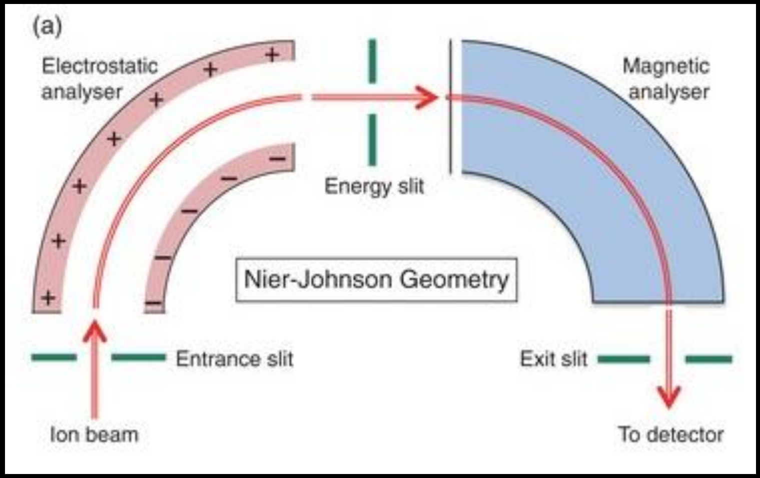
$$F_{Electic} = F_{centripetal}$$

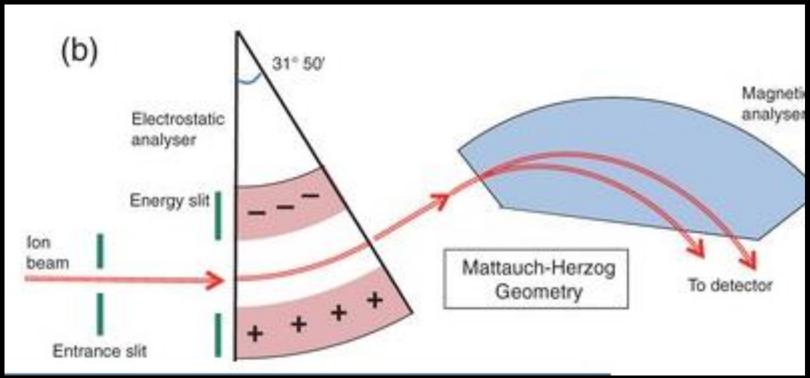
$$E\rho = \frac{mv^2}{q}$$

✓ **Difficult to bend energetic particles with raisonnable E field due to sparking**

➡ **Most used for low energy particles keV**

- Aston Nobel price (1919) : E+ B selection with a « mass spectrograph »
  - ✓ identification Stable isotopes : $^{20-22}Ne$; $^{35-37}Cl$ & mass measurement





Magnetic Separation:

$$\mathbf{F}_{\text{Magnetic}} = \mathbf{F}_{\text{centripetal}}$$

$$\mathbf{F}_{\text{magnetic}} = \text{q}\ \mathbf{v}\ \mathbf{B}$$

$$B\rho = \frac{mv}{q}, \rightarrow \text{Magnetic Rigidity}$$

Beam rigidity quantifies how difficult it is to bend the beam and is given by the total momentum divided by the total charge

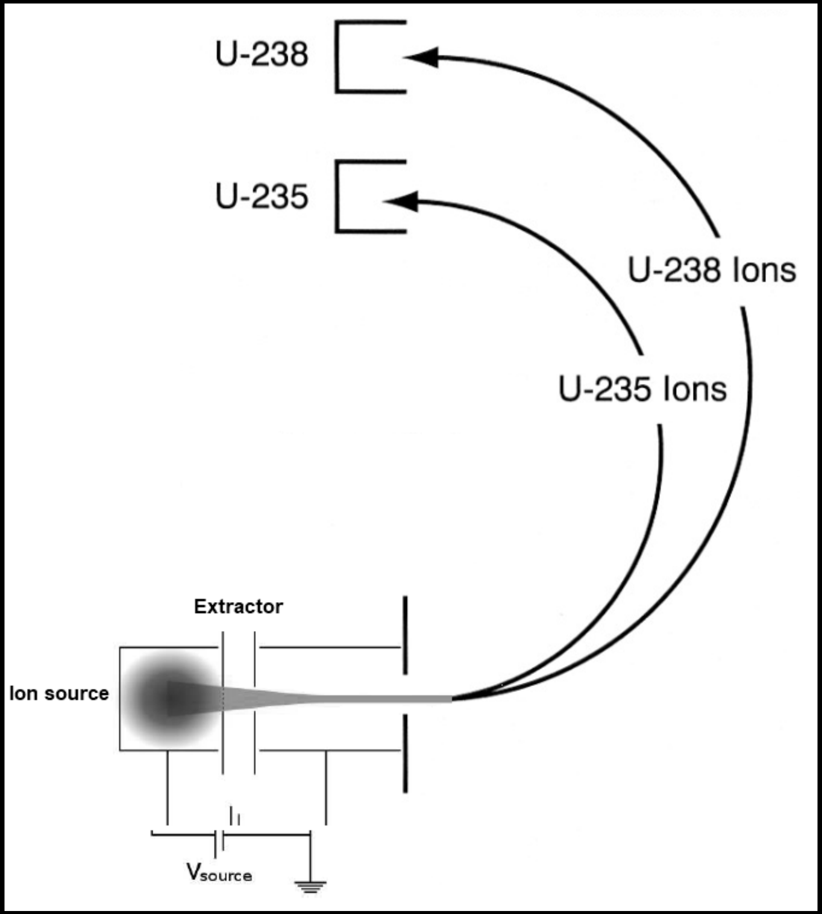
Wien Filter: $\mathbf{F}_{\text{electic}} = \mathbf{F}_{\text{magnetic}}$

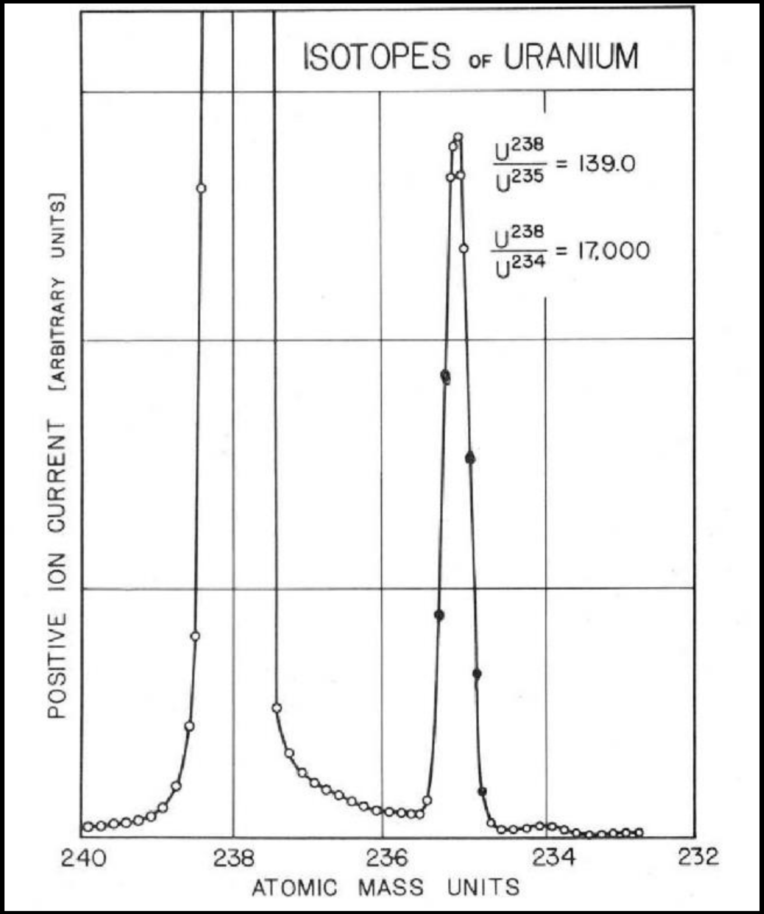
$$\text{v} = \text{E/B with E} \perp \text{B}$$

$$\text{m/q} = \frac{2Ek}{qv^2}$$

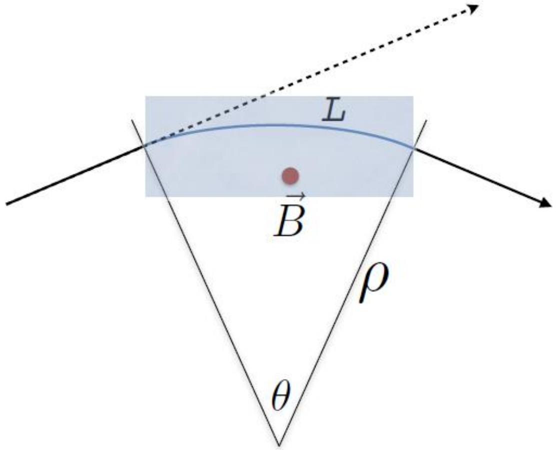
The simplest m/q magnetic spectrometer : 1 dipole magnet

- 40’s: Manhattan project U-235/U-238 enrichment (B selection)
- Dipole →mass dispersion





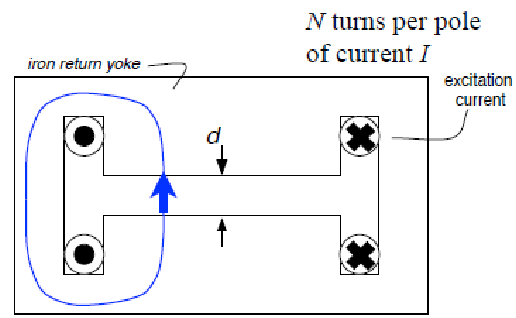
Bending through Dipole Field



$$\theta = \frac{L}{\rho} = \frac{B \cdot L}{(B\rho)} = \frac{q \cdot B \cdot L}{p}$$

- Iron-dominated magnetic fields
  - iron will "saturate" at about 2 Tesla

$$B = \frac{2\mu_0 N \cdot I}{d}$$

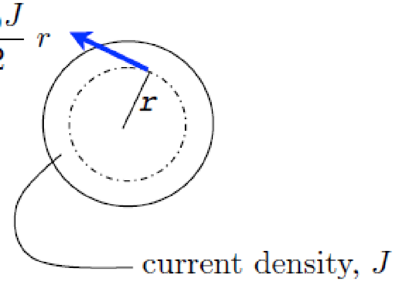


J_{eng} ~ 400 A/mm^2

Nb-Ti up to	8 T
Nb_3Sn up to	13 T
HTS up to	20 T

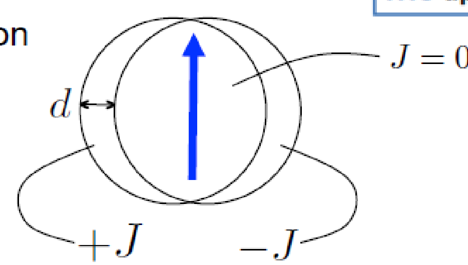
- High-field superconducting magnets
  - field determined by distribution of currents

$$B_\theta = \frac{\mu_0 J}{2} r$$



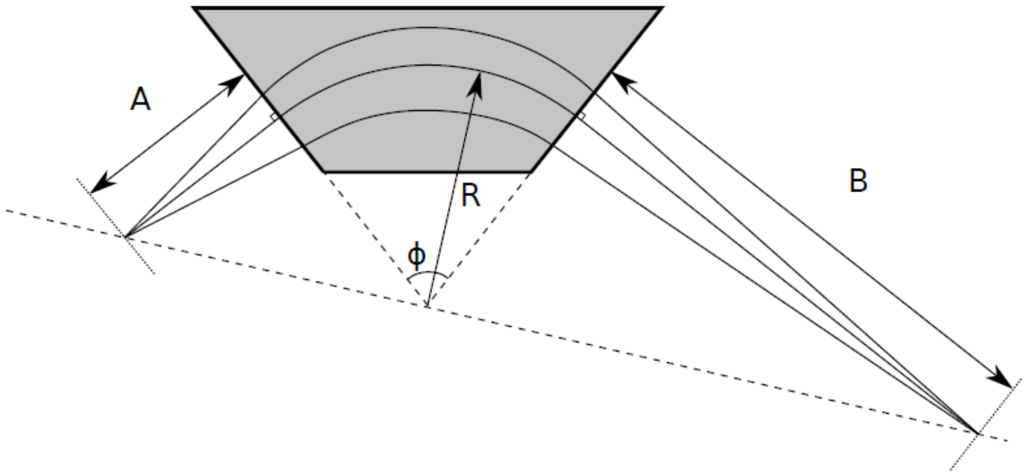
"Cosine-theta" distribution

$$B_x = 0, \quad B_y = \frac{\mu_0 J}{2} d$$

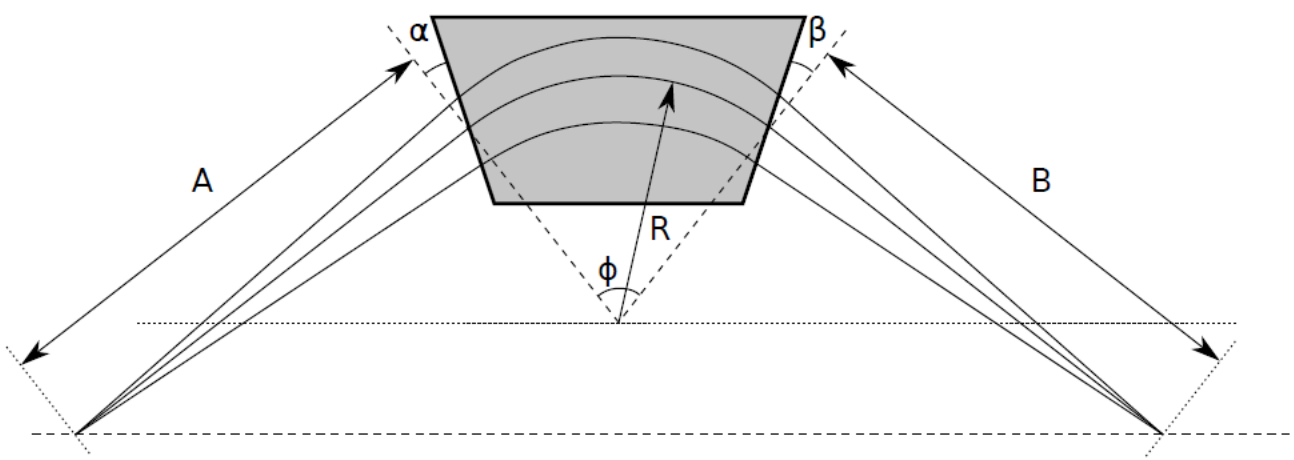


The dipole elements also have focusing/defocusing properties.

With edges perpendicular to the optical axis (edge angle 0◦) focuses the beam in the bending plane (x). There is no focusing action in the y direction.



If the magnet edge angles deviate from 90◦, the focusing power in the x direction can be adjusted. If the edge angle is made positive (as shown), there is weaker focusing in the x direction. If the angle is negative, there is stronger focusing in the x direction.

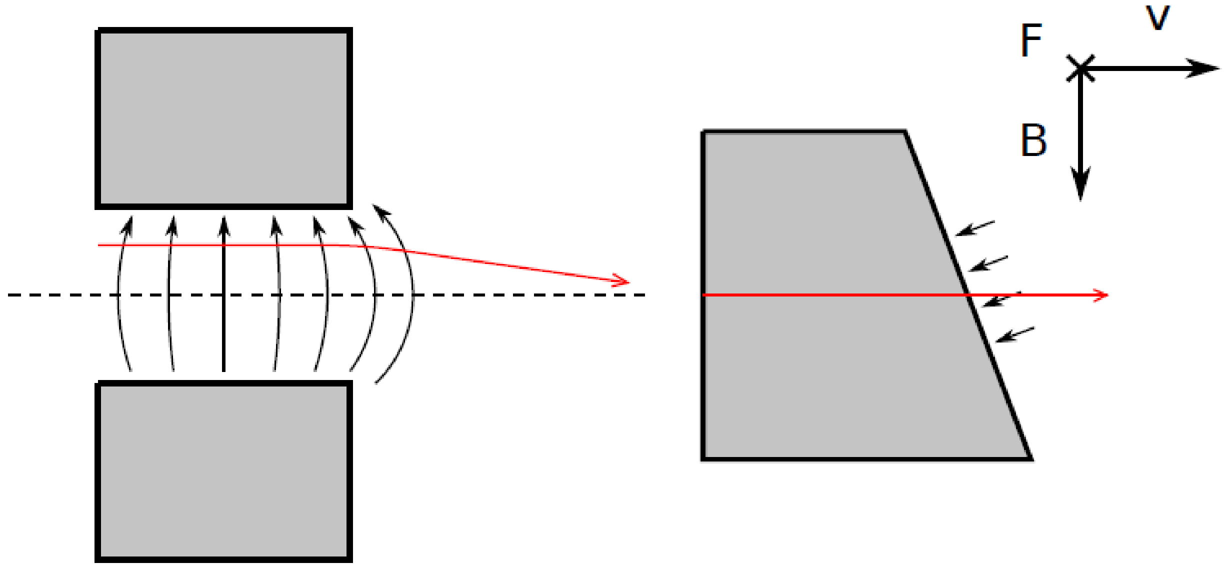


Changing the edge angle also has an important effect in the y direction:

if the angles are positive, the fringing field of the magnet will focus the beam in the y direction

Overall, this means that the focusing in the x direction can be traded for y focusing. The focal length from the edge focusing is given by.

$$f_Y = \frac{R}{\tan \alpha}$$



Dipôle : Traitement général

α	45	deg
R	1000	mm
gap	70	mm
β entrée	0	deg
β sortie	0	deg

K1	0,3
K2	4
Indice	0

ar	0,78539816	a1	-0,40985932
te	0	a2	-3,04647909
ts	0	a3	0,63661977
ca	0,70710678	Q	-1,03415799
sa	0,70710678	R	-0,10765524
delta	1	D	-1,09442448
par1	7,0711E+11		
par2	707106780	par5	-707,106781
par3	0,00070711		4
par4	-1,41421356	-414,213562	2414,21356

Arête	414,213562	mm	Ro Theta	785,398163	mm
Equifocale	2414,21356	mm	Cd (dp/p)	2	mm/pm
Foc. Objet	1E+12	mm	Foc. Image	1000	mm
			Cd (dp/p)	1	mm/pm

ATTENTION : Erreur de calcul sur les distances focales pour aimants à indice

	Correction 1er niveau			Correction 2ème niveau	
	radian	degré		radian	degré
ψ entrée	0,021	1,20321137		0,021	1,20321137
ψ sortie	0,021	1,20321137		0,021	1,20321137

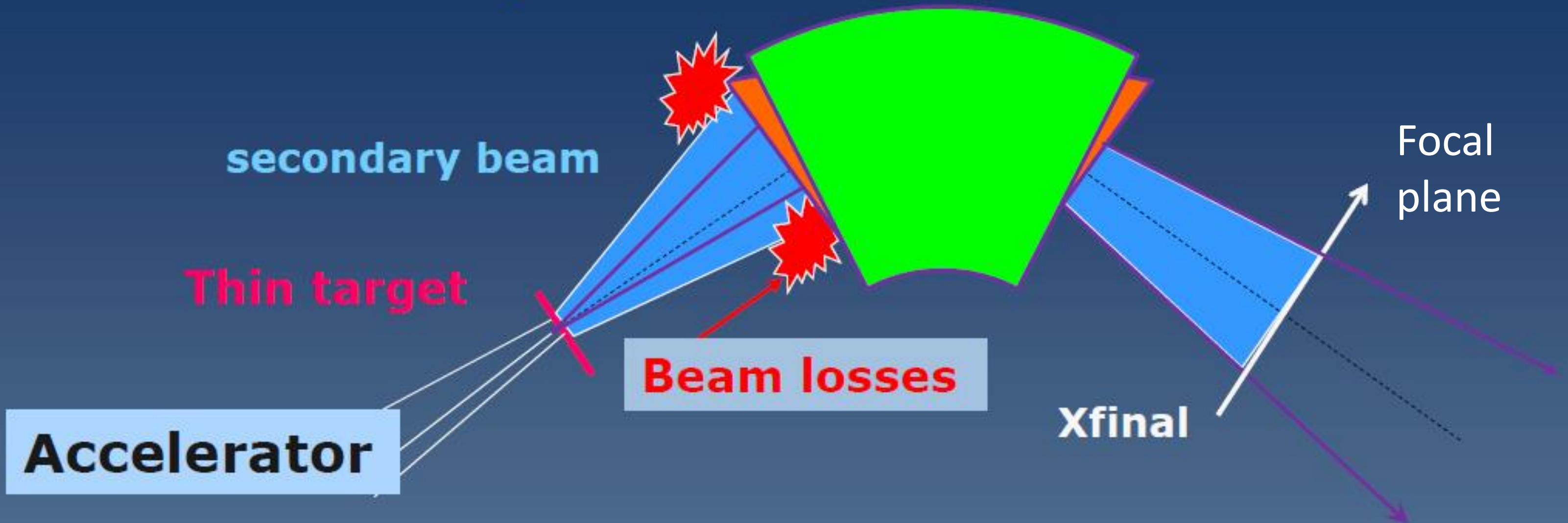
Dipôle à T11 = 0 (sans indice)		
α	45	deg
R	1000	mm
β (e/s)	0	deg
Focale	1000	mm

Dipôle secteur (sans indice)		
α	45	deg
R	1000	mm
ε (e/s)	0	deg
Focale	2414,21356	mm
Cd (dp/p)	2	mm/pm
ψ entrée (1)	0,021	1,20321137
ψ sortie (1)	0,021	1,20321137
ψ entrée (2)	0,021	1,20321137
ψ sortie (2)	0,021	1,20321137

Dipôle à double focalisation (sans indice)		
α	45	deg
R	1000	mm
ε (e/s)	11,7009195	deg
Focale	4828,42712	mm
Cd (dp/p)	4	mm/pm
ψ entrée (1)	0,02232769	1,27928238
ψ sortie (1)	0,02232769	1,27928238
ψ entrée (2)	0,02193926	1,25702674
ψ sortie (2)	0,02193926	1,25702674

Dipôle à T11 = T33 = 0 (sans indice)		
α	45	deg
R	1000	mm
tan(ε)	0,20612762	*racine 1*
ε (e/s)	11,6471149	deg
Focale	2212,03854	mm
Cd (dp/p)	1,99058892	mm/pm
tan(ε)	-1,65848937	*racine 2*
ε (e/s)	-58,9117733	deg
Focale	-420,386128	mm
Cd (dp/p)	0,19984222	mm/pm
tan(ε)	1,86222106	*racine 3*
ε (e/s)	61,764505	deg
Focale	-462,221908	mm
Cd (dp/p)	-0,28605761	mm/pm

2 problems with 1 dipole magnet :
Acceptance & identification



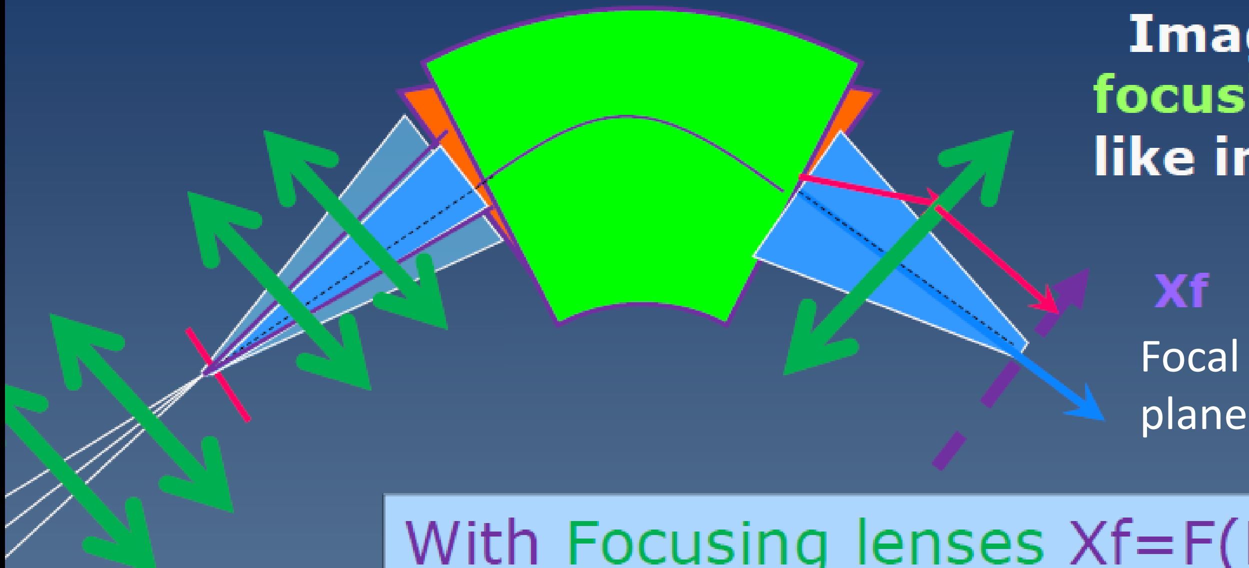
-1: Many particles are lost in the magnet (very bad)

-2: Trajectories are complex (bad)

Xfinal =f(Bρ , θi, φi , X0,Y0)

- Final position *xf* depend on the
  - Bρ (good for identification or separation)
  - position & Angle after the reaction (bad)

Beam divergence after target
2 problems solved with focusing lenses



Imagine than
focusing lenses exist
like in light optics

With Focusing lenses $X_f=F(B\rho,$ ~~θ_i~~, ~~ϕ_i~~, ~~X_0~~, ~~Y_0~~$)$

less unknowns ! **Less beam losses**!!

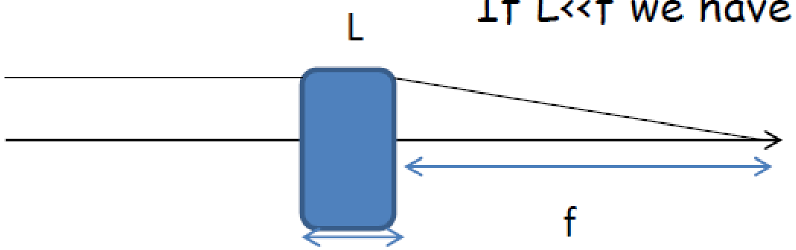
The trajectoires are independant of the angles θ_i, ϕ_i

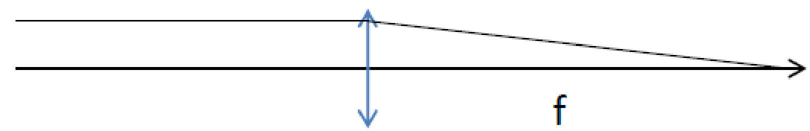
And the initial position is $x_0=0$, $y_0=0$

$X_f=F(B\rho,$ ~~θ_i~~, ~~ϕ_i~~, ~~X_0~~, ~~Y_0~~ $)$

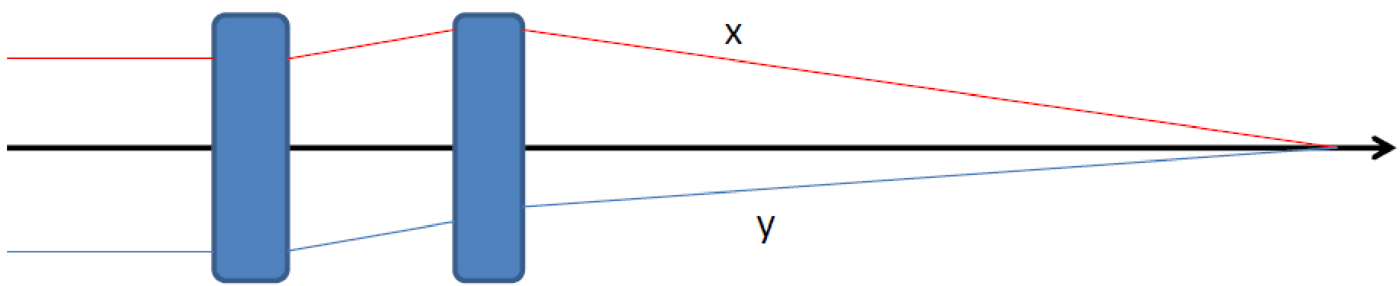
Focusing in both planes : doublets, triplets

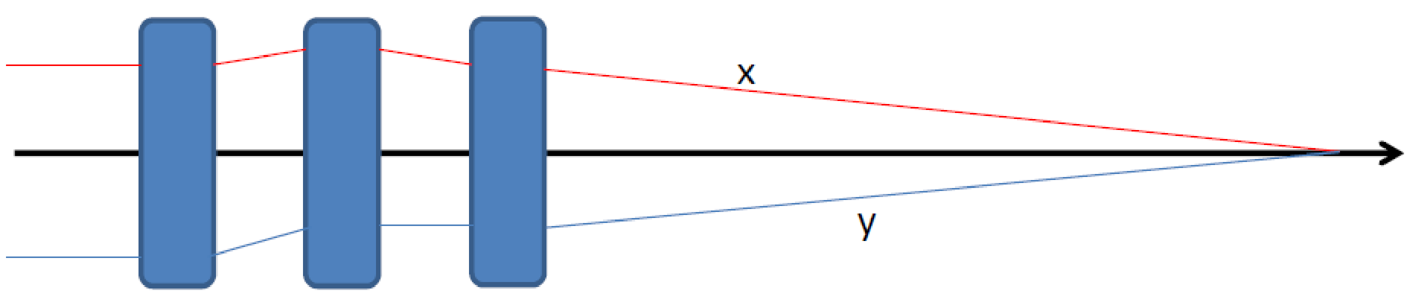
If L<<f we have the 'Thin Lens Model'





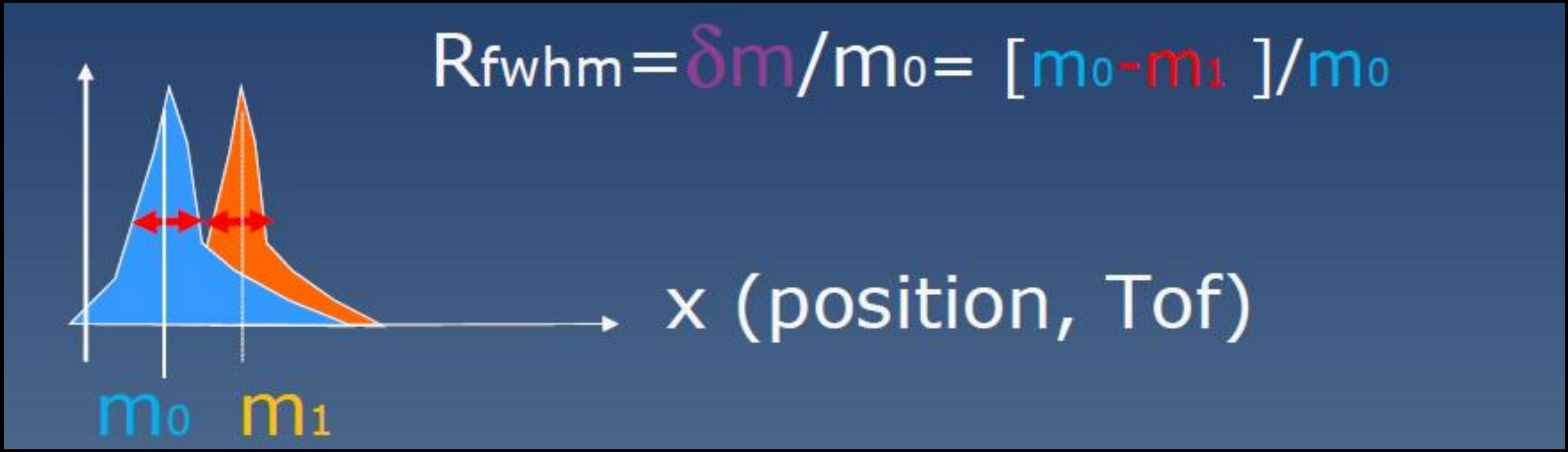
But how to have a Net Focusing effect in the two plans? : DOUBLETS/TRIPLETS

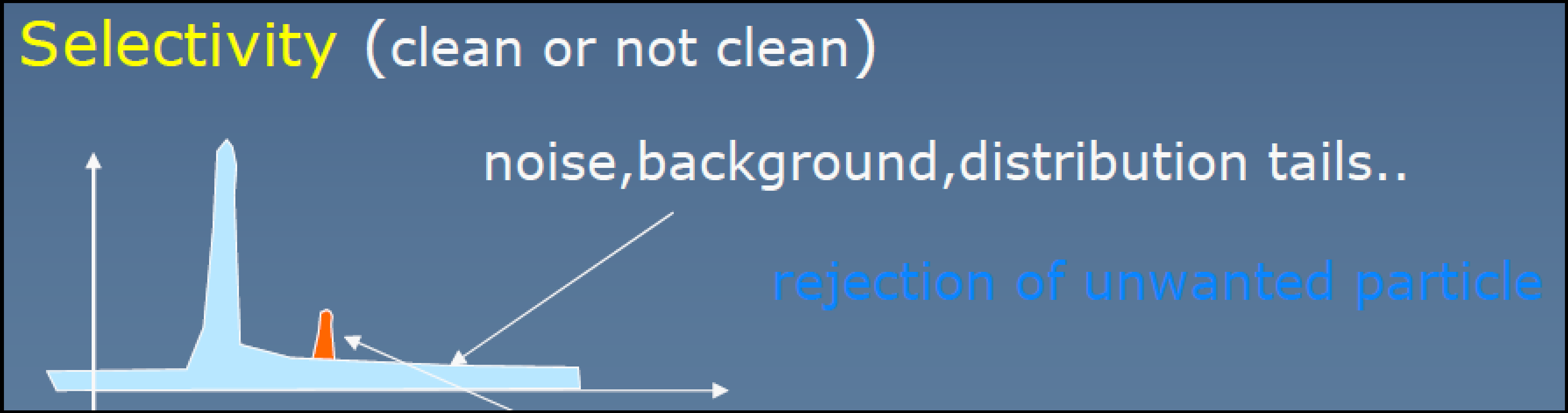




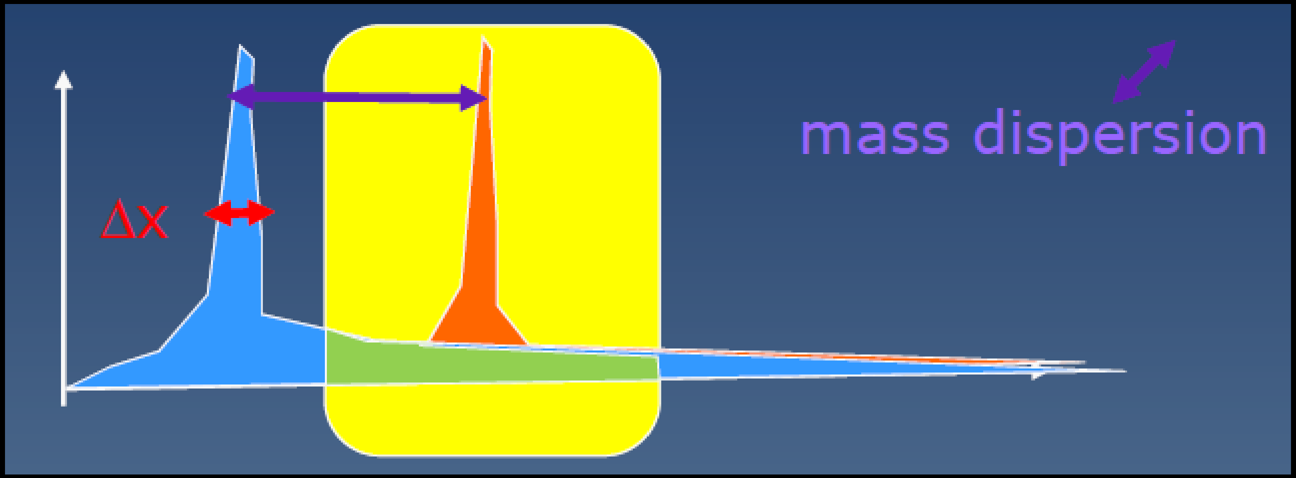
Resolving power

The term resolving power is the ability of a spectrometer to resolve adjacent peaks in a mass spectrum and is often used interchangeably with resolution. The separation of peaks for singly charged ions can be expressed as a mass difference δm





Resolution = Δx_{FWHM} / dx/dm, Resolving power = 1/Resolution

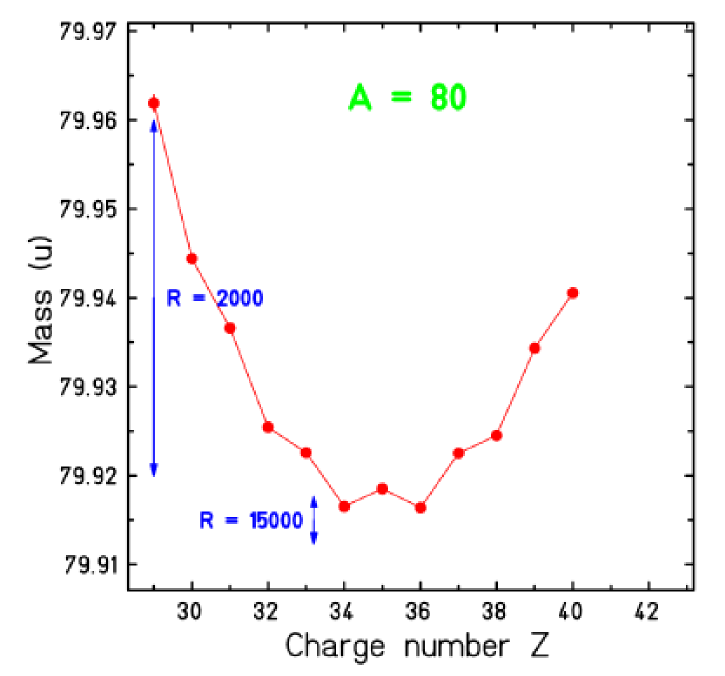


Mass dispersion usually expressed in meters (m) (SI):
cm/% (centimeters per 100%) ;
mm/‰

Notation :
- ✓ D_m
- ✓ dx/dm, physical meaning

Matricial notation (see later)
- ✓ (x|δ) Wollnik
- ✓ R16, T16, M16

- ✓ Resolving power R = $\frac{(x|\delta)}{\Delta x\ (FWHM)}$



Exercise 1:
Imagine a spectrometer with a dispersion of 30 cm/%
and beam width of 1 mm FWHM on the focal plan detector.

What is the resolving power R ?

a) 30
b) 30000
c) 1500

Beam optics (basics)

Already seen:

- ✓ Dispersion and focalisation with dipoles
- ✓ Focalisation with quadrupoles
- ✓ Resolution

Next concepts:

- **Particles coordinates**
- **Beam emittance**
- **Optical Matrices following Taylor expansion**
- **Angular Acceptance**
- **Bρ Acceptance**

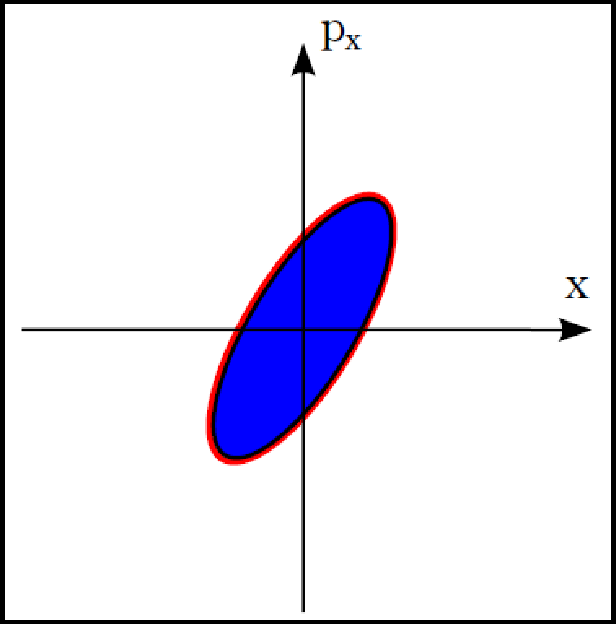
The Coordinates

Notations in the Literature is not consistent!

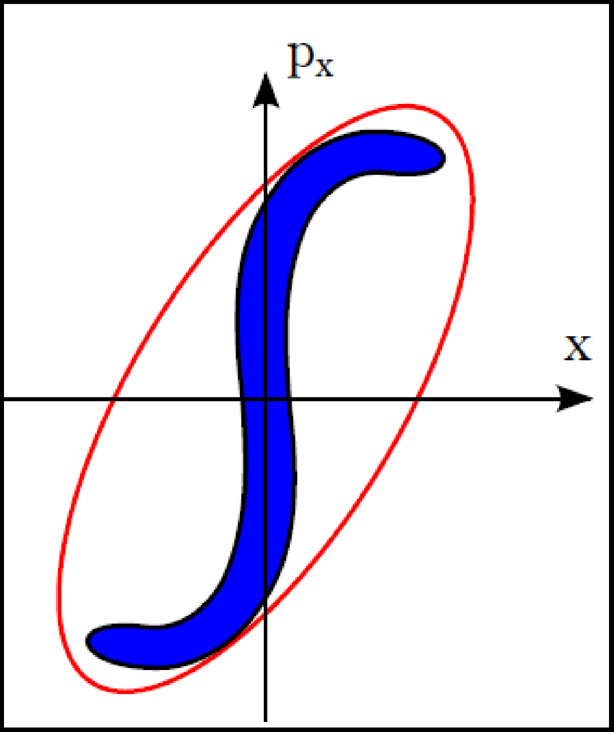
Wollnik GICOSY	Brown	TRANSPORT	COSY	Meaning
x	x	x	r1 = x	the horizontal displacement of the arbitrary ray with respect to the assumed central trajectory.
a	x'	θ	r2 = a = p_x/p_0	the angle this ray makes in the horizontal plane with respect to the assumed central trajectory.
y	y	y	r3 = y	the vertical displacement of the ray with respect to the assumed central trajectory
b	y'	φ	r4 = b = p_y/p_0	the vertical angle of the ray with respect to the assumed central trajectory
ℓ	ℓ		r5 = ℓ = $-(t - t_0)v_0\gamma/(1 + \gamma)$	the path length difference between the arbitrary ray and the central trajectory.
δ	δ	$dp/p = \frac{B\rho - B\rho_0}{B\rho_0}$		fractioned momentum deviation of the ray from the assumed central trajectory
δ_U			r6 = $\delta K = (K - K_0)/K_0$	energy difference ray with respect to the reference energy
δ_m			r7 = $\delta m = (m - m_0)/m_0$	mass difference ray with respect to the reference energy
δ_e			r8 = $\delta z = (z - z_0)/z_0$	charge difference ray with respect to the reference energy

Beam emittance

The emittance is defined as the six-dimensional volume limited by a contour of constant particle density in the (x, px, y, py, z, pz) phase space. This volume obeys the Liouville theorem and is constant in conservative fields



optical system

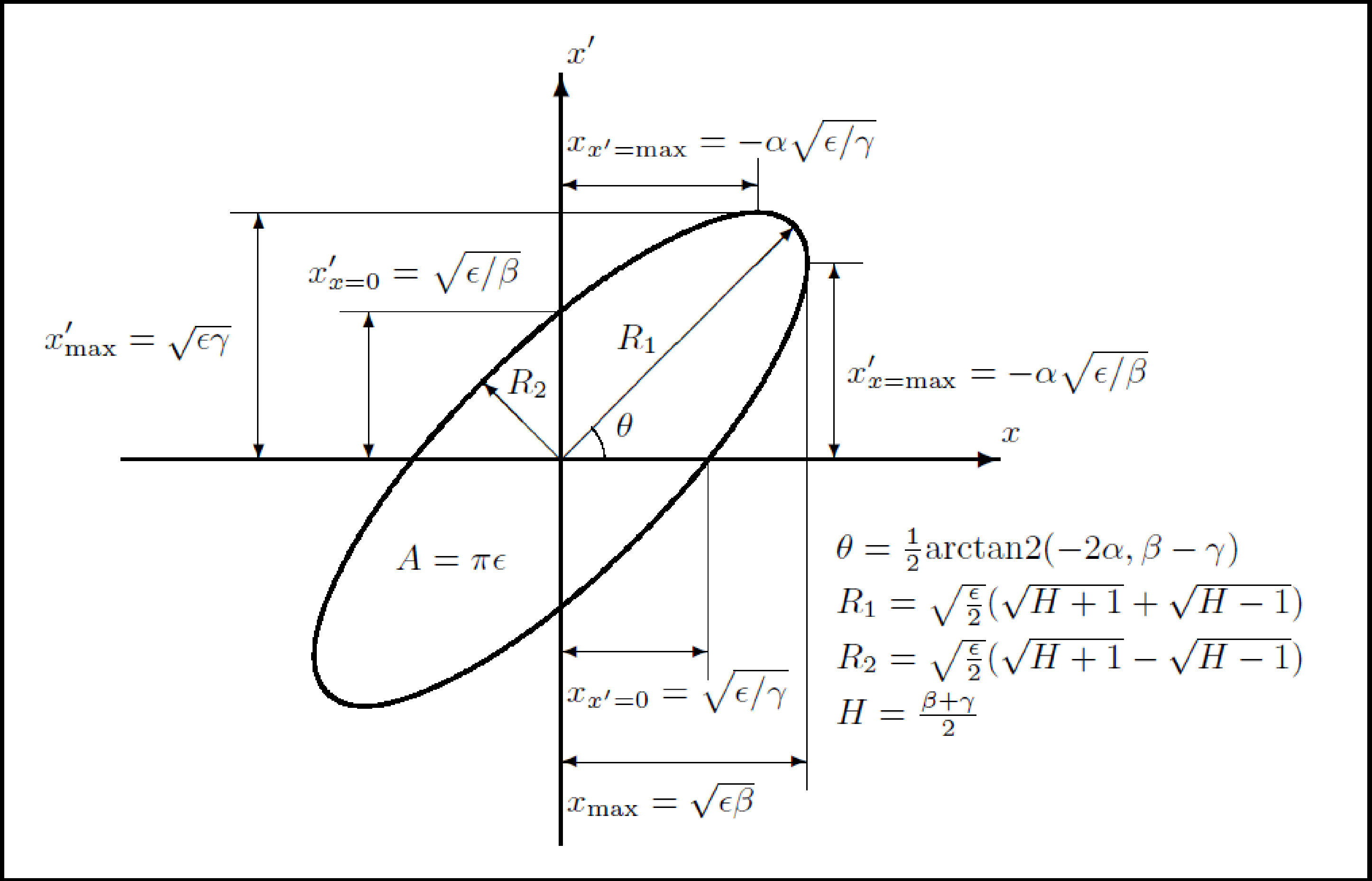


The area of the particle distribution is conserved but the area of the elliptical envelope increases.

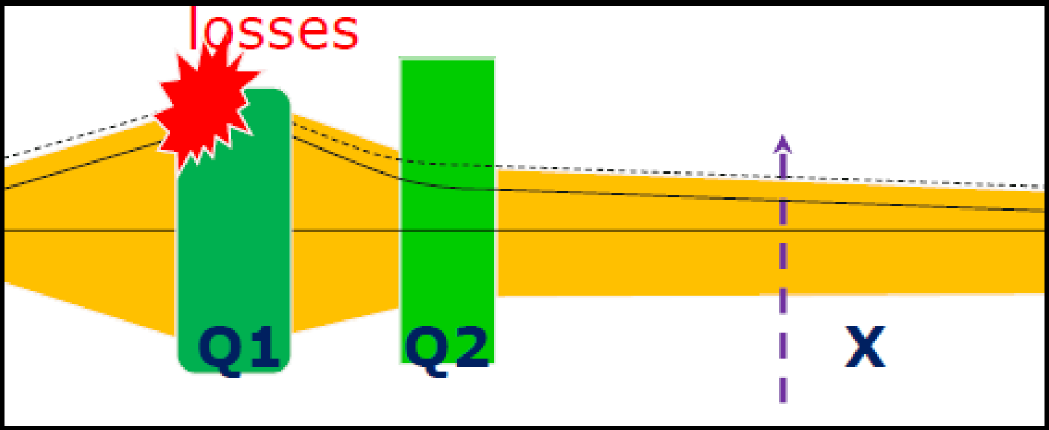
Beam emittance

$$\gamma x^2 + 2\alpha x x' + \beta x'^2 = \varepsilon \qquad \beta\gamma - \alpha^2 = 1 \qquad A = \pi\varepsilon = \pi R_1 R_2$$

ε is the two-dimensional transverse emittance, and α, β and γ are known as the Twiss parameters



The beam size : important for the design



Ellipse Area = $\pi(\det \sigma)^{1/2}$

Emittance $\varepsilon = \det \sigma$ is constant for fixed energy & conservative forces (Liouville's Theorem)

Note: ε shrinks (increases) with acceleration (deceleration);
Dissipative forces: ε increases in gases; electron, stochastic, laser cooling

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{21} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} = \varepsilon \begin{pmatrix} \beta & -\alpha \\ -\alpha & \gamma \end{pmatrix}$$

The percentage of bivariate normally distributed data covered by an ellipse whose axes have a length of *numberOfSigmas* · σ can be obtained by integration of the probability distribution function over an elliptical area.

$$\textit{percentage} = (1 - \exp(-\textit{numberOfSigmas}^2/2)) \cdot$$

This results in the following equation,

$$(x/\sigma_x)^2 + (y/\sigma_y)^2 = \textit{numberOfSigmas}^2.$$

where the *numberOfSigmas* is the radius of the "ellipse":

the *numberOfSigmas* =1 ellipse covers 39.3% of the data,
the *numberOfSigmas* =2 ellipse 86.5%,
and the *numberOfSigmas* =3 ellipse 98.9%.

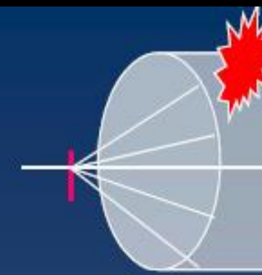
From the formula above we can show that if we want to cover *p* percent of the data, we have to chose *numberOfSigmas* as

$$\textit{numberOfSigmas} = \sqrt{(-2 \ln(1-p/100))}.$$

For covering 95% of the data we calculate *numberOfSigmas* = **2.45.**

$$\textbf{Resolving power (95\%)} = \frac{(x|\delta)}{\Delta x\ (2.45\ \sigma)}$$

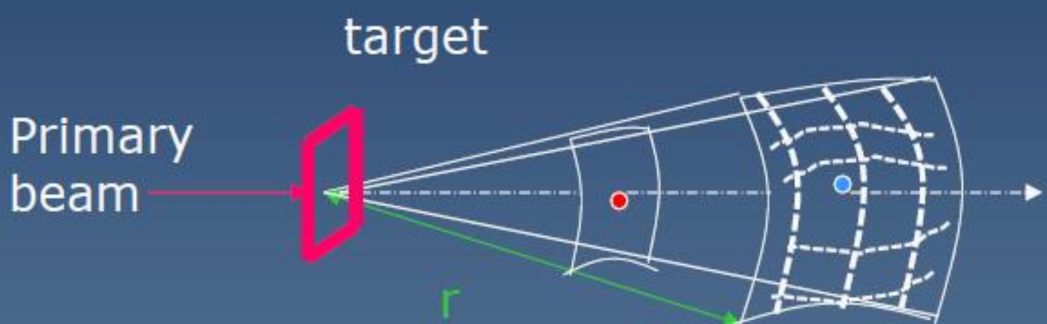
Angular acceptance



The reaction products exit from the target with an

Angular dispersion

Vacuum chamber limitation induces beam losses = less transmission



The acceptance is measured in steradian

$$d\Omega(strd) = \frac{dS}{r^2}$$

dS

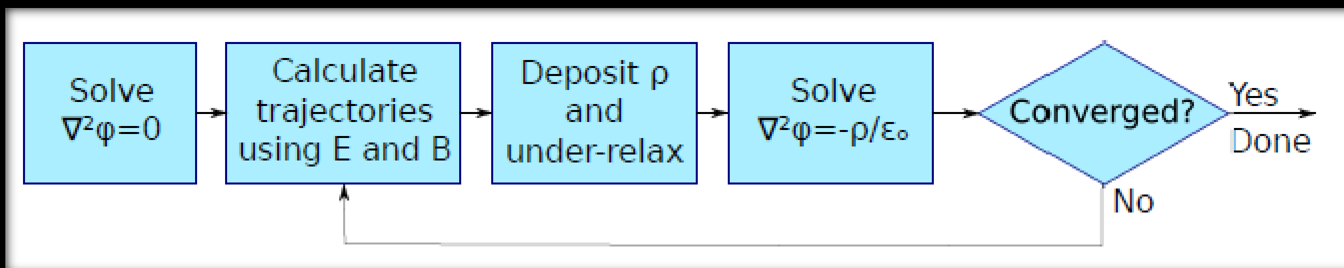
Bρ Acceptance = ± Xmax / R_{16}

Modelling of ion optical transport lines

1. Trajectories : exact equations

integrate the particle equation of motion using mesh based maps for E and B fields [field map 3D]

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F} = q(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B})$$



$$\frac{d}{ds}\left[m\gamma\dot{x}\right] = m\gamma\dot{s}(1+\frac{x}{\rho}) + q(t'E_x + y'B_s - \dot{s}(1+\frac{x}{\rho})\cdot B_y)$$

$$\frac{d}{ds}\left[m\gamma\dot{y}\right] = q(t'E_y + (1+\frac{x}{\rho})\cdot B_x - x'\cdot B_s)$$

$$\frac{d}{ds}\left[m\gamma\dot{s}(1+\frac{x}{\rho})\right] = -\frac{m\gamma\dot{x}}{\rho} + q(t'E_s + x'\cdot B_y - y'\cdot B_x)$$

Examples of codes : ZGOUBY

But generally we can do simpler : Matrix approach

Modelling of ion optical transport lines

Taylor expansion in x, a, y, b and δ

$$x_1 = (x|x)\, x_0 + (x|a)\, a_0 + (x|\delta)\delta + (x|x^2)x_0^2 + (x|xa)\, x_0 a_0 + (x|a^2)a_0^2$$

$$(x|x\delta)\, x_0 + (x|a\delta)\, a_0\delta + (x|\delta^2)\delta^2 + (x|y^2)y_0^2 + (x|yb)\, y_0 b_0 + (x|b^2)b_0^2$$ + higher orders

First order

$$(x|\ \ldots) = \frac{\partial}{\partial x}$$

$$Higher\ orders : e.g.\ (x|a^2) = \frac{\partial x}{\partial a \partial a} = T_{122}$$

Transfer matrix formalism

6x6 Matrix
representing first
optic element
(usually a Drift)

$$x_n = T_n T_{n-1} \dots T_0 x_0$$

Ray at final
Location n

Ray at initial
Location 0
(e.g. a target
or slits)

Complete system is represented in first order by one Matrix Rsystem = $T_n\ T_{n-1} \dots T_0$

Transfer matrix formalism

Most crucial parameters :

$$
T = \begin{pmatrix}
(x|x) & (x|a) & (x|y) & (x|b) & (x|l) & (x|\delta) \\
(a|x) & (a|a) & (a|y) & (a|b) & (x|l) & (a|\delta) \\
(y|x) & (y|a) & (y|y) & (y|b) & (x|l) & (y|\delta) \\
(b|x) & (b|a) & (b|y) & (b|b) & (x|l) & (a|\delta) \\
(l|x) & (l|a) & (l|y) & (l|b) & (x|l) & (l|\delta) \\
(\delta|x) & (\delta|a) & (\delta|y) & (\delta|b) & (x|l) & (\delta|\delta)
\end{pmatrix}
$$

$$T_{11} = magnification\ in\ horizontal$$

$$T_{16} = dispersion\ in\ momentun = dispersion\ in\ B\rho$$

$$T_{33} = magnification\ in\ vertical$$

$$T_{12} = angular\ dependance\ in\ horizontal$$

$$T_{34} = angular\ dependance\ in\ vertical$$

Dipôle : Traitement général

α	54	deg
R	1500	mm
gap	50	mm
β entrée	0	deg
β sortie	35	deg

K1	0,3
K2	4
Indice	0

Arête	764,288174	mm	Ro Theta	1413,71669	mm
Equifocale	7209,91164	mm	Cd (dp/p)	8,53230231	mm/pm
Foc. Objet	1E+12	mm	Foc. Image	2218,36267	mm
			Cd (dp/p)	3,05331427	mm/pm

ATTENTION : Erreur de calcul sur les distances focales pour aimants à indice

	Correction 1er niveau			Correction 2ème niveau	
	radian	degré		radian	degré
ψ entrée	0,01	0,5729578		0,01	0,5729578
ψ sortie	0,01622397	0,92956508		0,01576957	0,90352955

ar	0,9424778	a1	-0,50173564
te	0	a2	-2,04177113
ts	0,70020754	a3	0,53051648
ca	0,58778525	Q	-0,70856134
sa	0,80901699	R	-0,08984201
delta	1	D	-0,34766813
par1	5,8779E+11		
par2	264963552	par5	-1213,52549
par3	0,00026496		4,32089936
par4	-1,7420503	-635,232665	7209,91164

Dipôle à T11 = 0 (sans indice)		
α	54	deg
R	1500	mm
β (e/s)	0	deg
Focale	1089,81379	mm

Dipôle secteur (sans indice)		
α	54	deg
R	1500	mm
ε (e/s)	0	deg
Focale	2943,91576	mm
Cd (dp/p)	3	mm/pm
ψ entrée (1)	0,01	0,5729578
ψ sortie (1)	0,01	0,5729578
ψ entrée (2)	0,01	0,5729578
ψ sortie (2)	0,01	0,5729578

Dipôle à double focalisation (sans indice)		
α	54	deg
R	1500	mm
ε (e/s)	14,2927863	deg
Focale	5887,83152	mm
Cd (dp/p)	6	mm/pm
ψ entrée (1)	0,01094837	0,62729536
ψ sortie (1)	0,01094837	0,62729536
ψ entrée (2)	0,0108368	0,6209029
ψ sortie (2)	0,0108368	0,6209029

Dipôle à T11 = T33 = 0 (sans indice)		
α	54	deg
R	1500	mm
tan(ε)	0,25206223	*racine 1*
ε (e/s)	14,1473961	deg
Focale	2574,38697	mm
Cd (dp/p)	2,96853344	mm/pm
tan(ε)	-1,33128437	*racine 2*
ε (e/s)	-53,0877978	deg
Focale	-780,546141	mm
Cd (dp/p)	0,41519128	mm/pm
tan(ε)	1,58095777	*racine 3*
ε (e/s)	57,6855026	deg
Focale	-911,648613	mm
Cd (dp/p)	-0,71333313	mm/pm

Exercise 2:

For covering 95% of the beam ellipse data which value of sigma in ΔX we should use for calculating the resolving power?

a) **1 σ**
b) **2.35 σ (FWHM)**
c) **2.45 σ**

Supplemental slides

Transfer matrix formalism

Following Taylor expansion the trajectory component Xi after propagation through an ion optical element can be calculated from

$$X_i = \sum_j Y_j \left\{ (X_i \mid Y_j) + \sum_k \frac{Y_k}{2} \left\{ (X_i \mid Y_j Y_k) + \sum_l \frac{Y_l}{3} \{ (X_i \mid Y_j Y_k Y_l) + \cdots \} \right\} \right\},$$

where Yi are the components of the trajectory before the ion optical element, and (Xi | Yj), (Xi | YjYk), (Xi | YjYkYl), . . . are the first-order, second-order, third-order, . . . transfer coefficients

This can be described as matrix–vector multiplication with :

6×6 matrix in first order
6×6^2 matrix in second order,
6×6^3 matrix in third order, etc.

Transfer matrix formalism

$$\begin{bmatrix} x \\ x' \\ y \\ y' \\ l \\ \delta \end{bmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} & T_{16} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} & T_{26} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} & T_{36} \\ T_{41} & T_{42} & T_{43} & T_{44} & T_{45} & T_{46} \\ T_{51} & T_{52} & T_{53} & T_{54} & T_{55} & T_{56} \\ T_{61} & T_{62} & T_{63} & T_{64} & T_{65} & T_{66} \end{pmatrix} \begin{bmatrix} x_0 \\ x'_0 \\ y_0 \\ y'_0 \\ l_0 \\ \delta_0 \end{bmatrix}$$

$$\mathrm{T} = \begin{pmatrix} (x|x) & (x|a) & (x|y) & (x|b) & (x|l) & (x|\delta) \\ (a|x) & (a|a) & (a|y) & (a|b) & (x|l) & (a|\delta) \\ (y|x) & (y|a) & (y|y) & (y|b) & (x|l) & (y|\delta) \\ (b|x) & (b|a) & (b|y) & (b|b) & (x|l) & (a|\delta) \\ (l|x) & (l|a) & (l|y) & (l|b) & (x|l) & (l|\delta) \\ (\delta|x) & (\delta|a) & (\delta|y) & (\delta|b) & (x|l) & (\delta|\delta) \end{pmatrix}$$