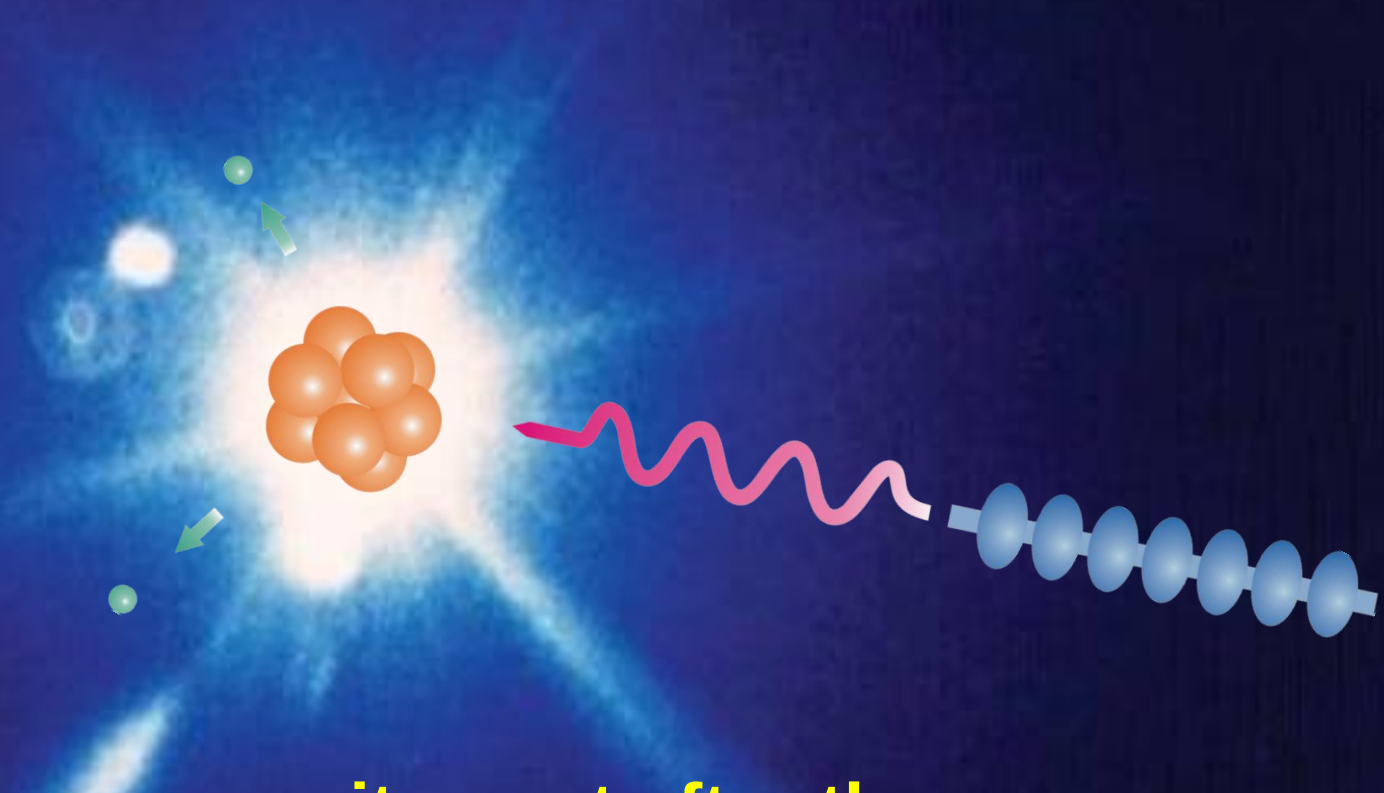


VUV excitation of mass selected clusters at the free electron laser FLASH



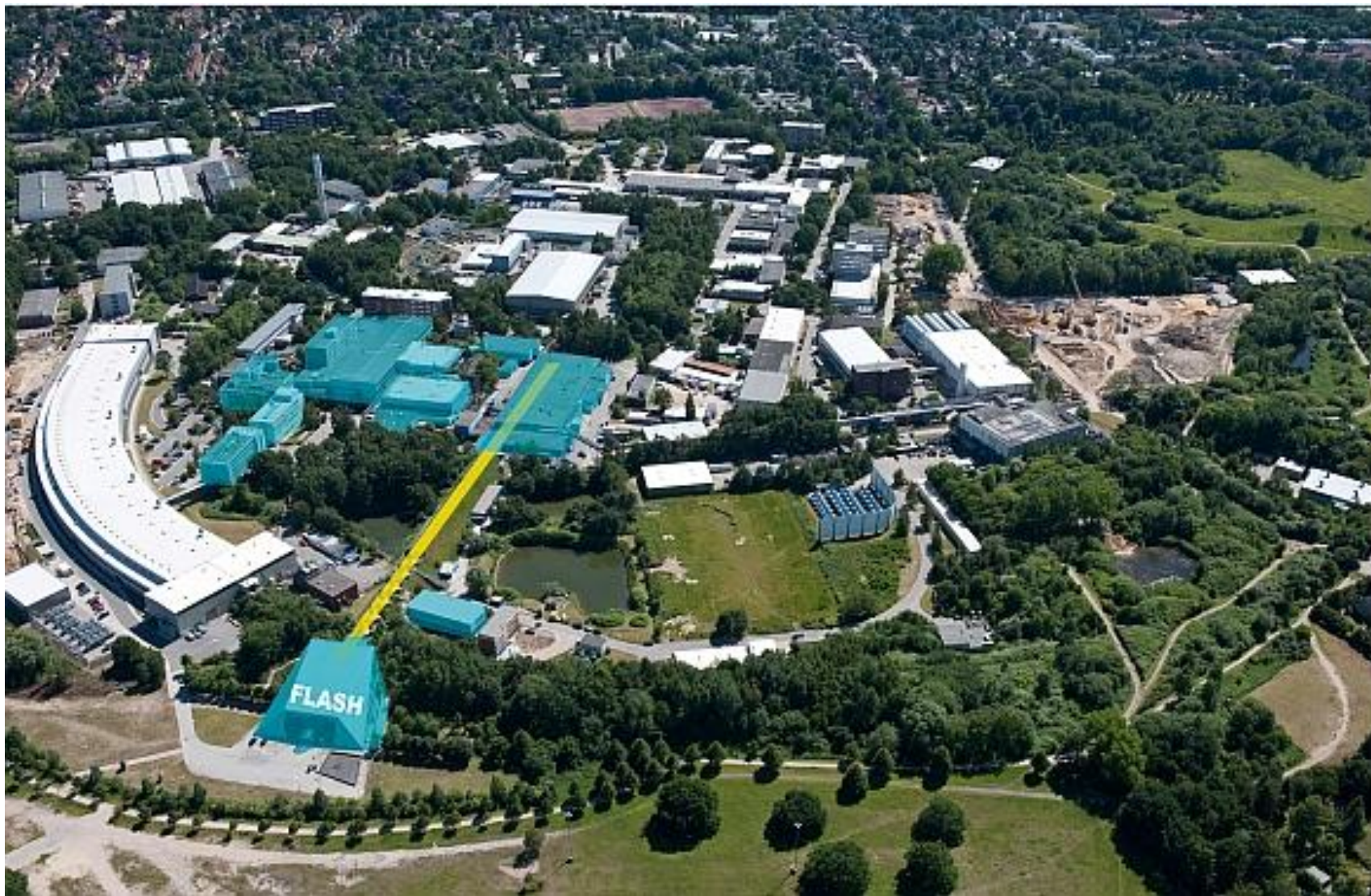
**excitement after the measurement
campaign at FLASH in Hamburg**

for the lecture start with slide no 12

FLASH 3 years ago

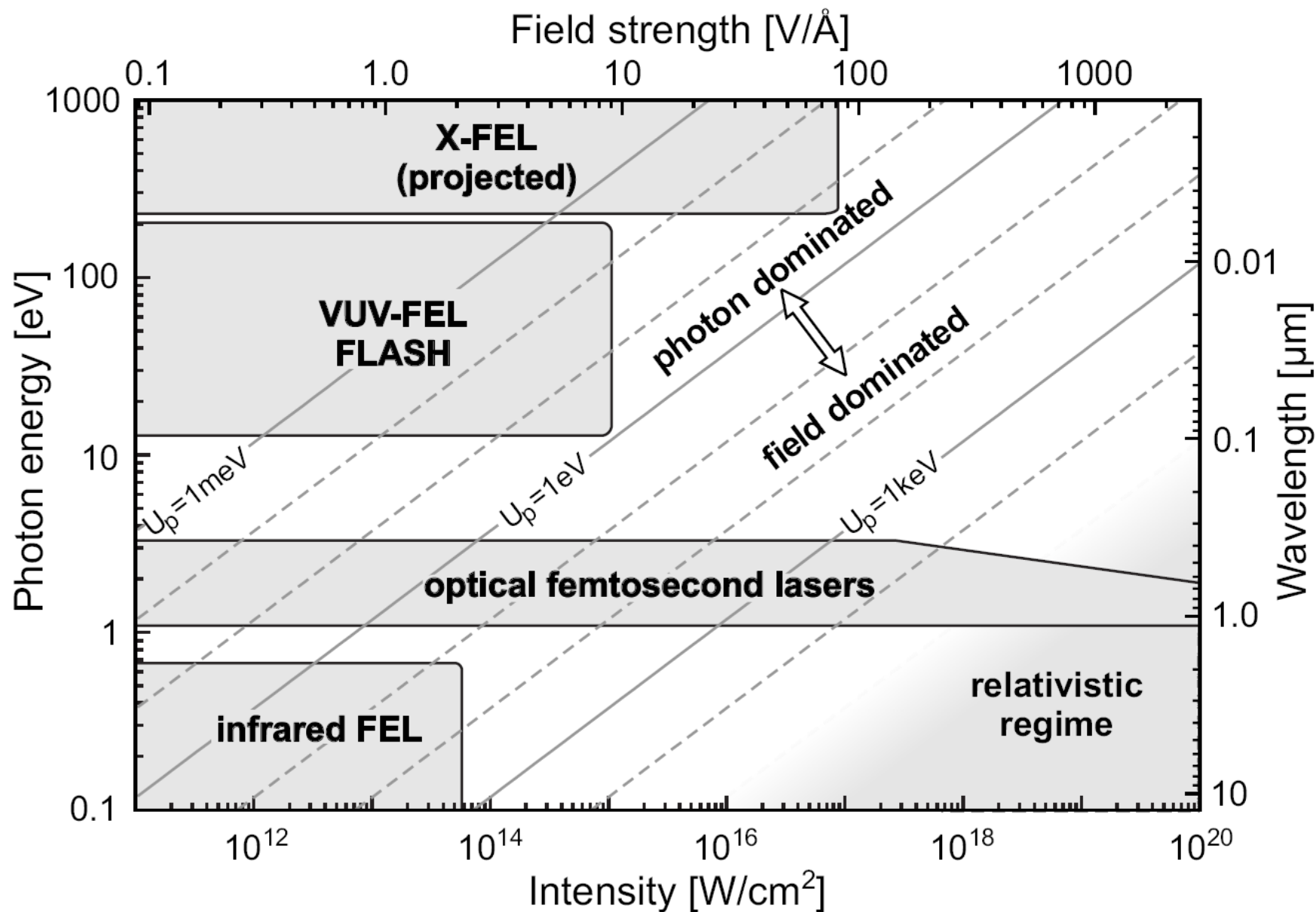


FLASH today

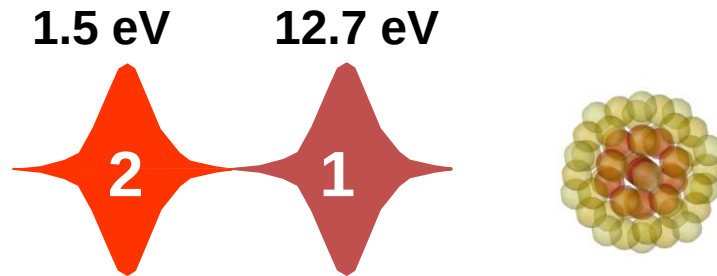


free electron laser FLASH up to 260 eV or down to 4.8 nm

Laser intensity regimes

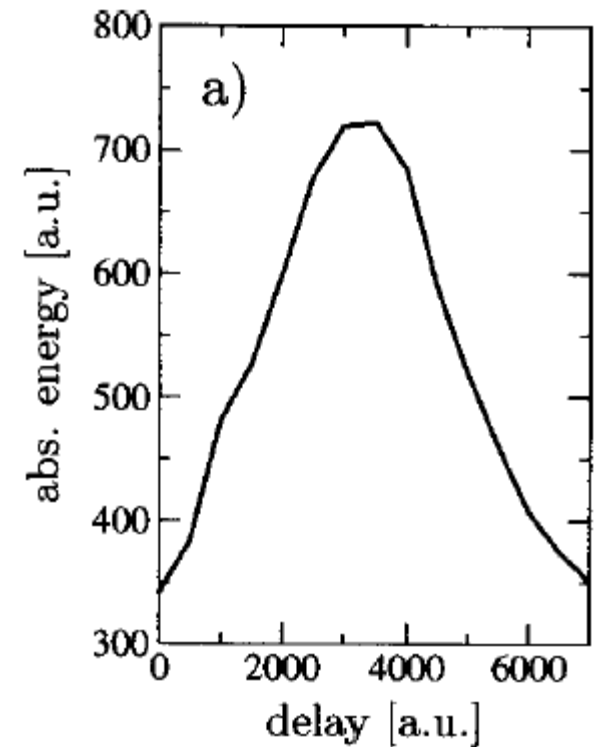


example 1: *metallization* of rare gas clusters with the FEL



1st VUV pulse(FEL): inner ionization

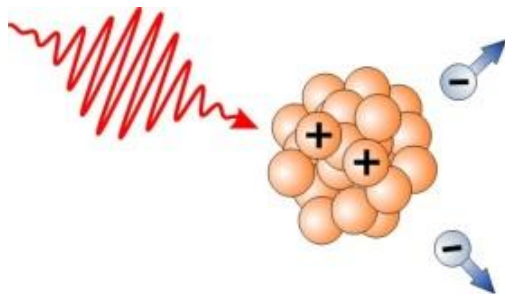
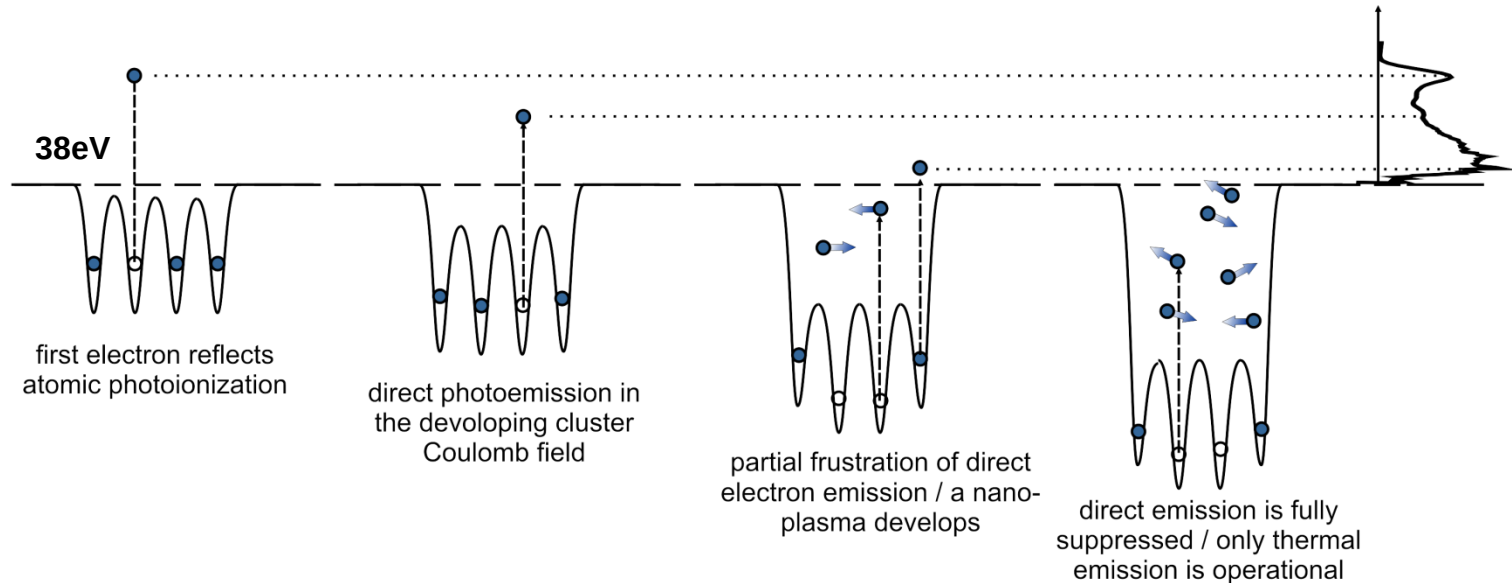
2st IR pulse: coupling to collective resonance



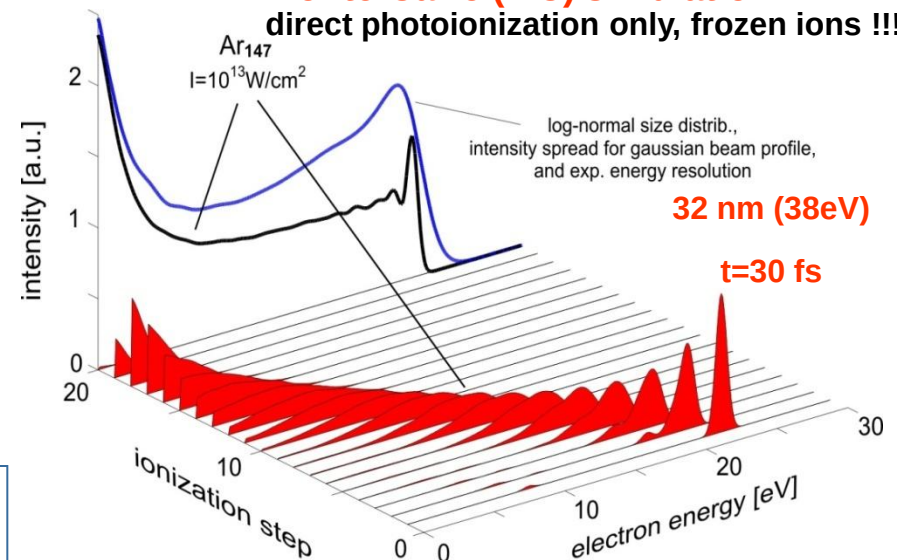
Theory: Ch. Siedschlag and J.M. Rost. Phys. Rev. A 71:031401, 2005

Experiments: Möller, Bostedt et al.

multistep ionization

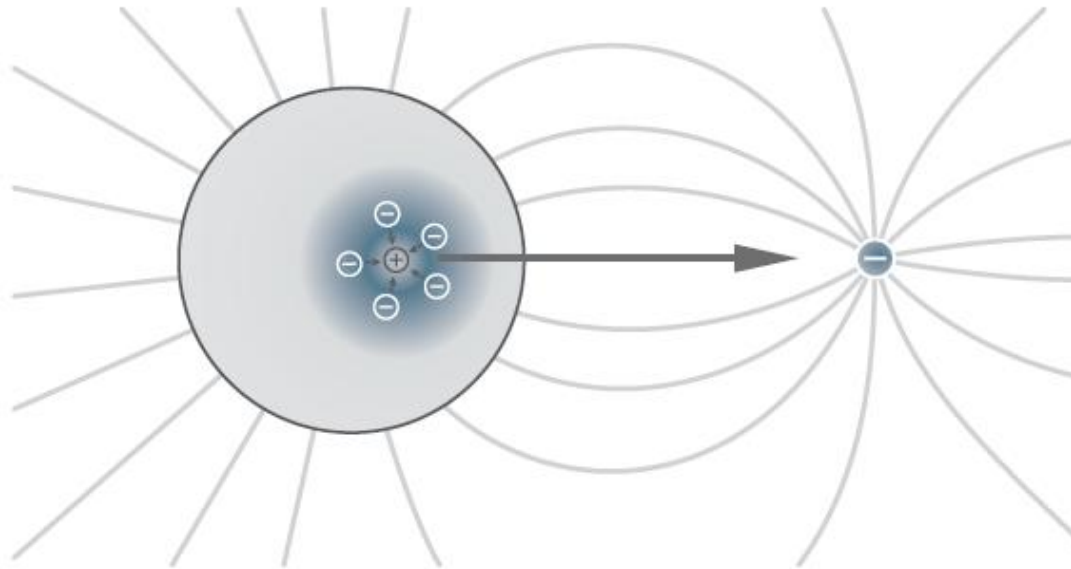


Monte-Carlo (MC) simulation:
direct photoionization only, frozen ions !!!



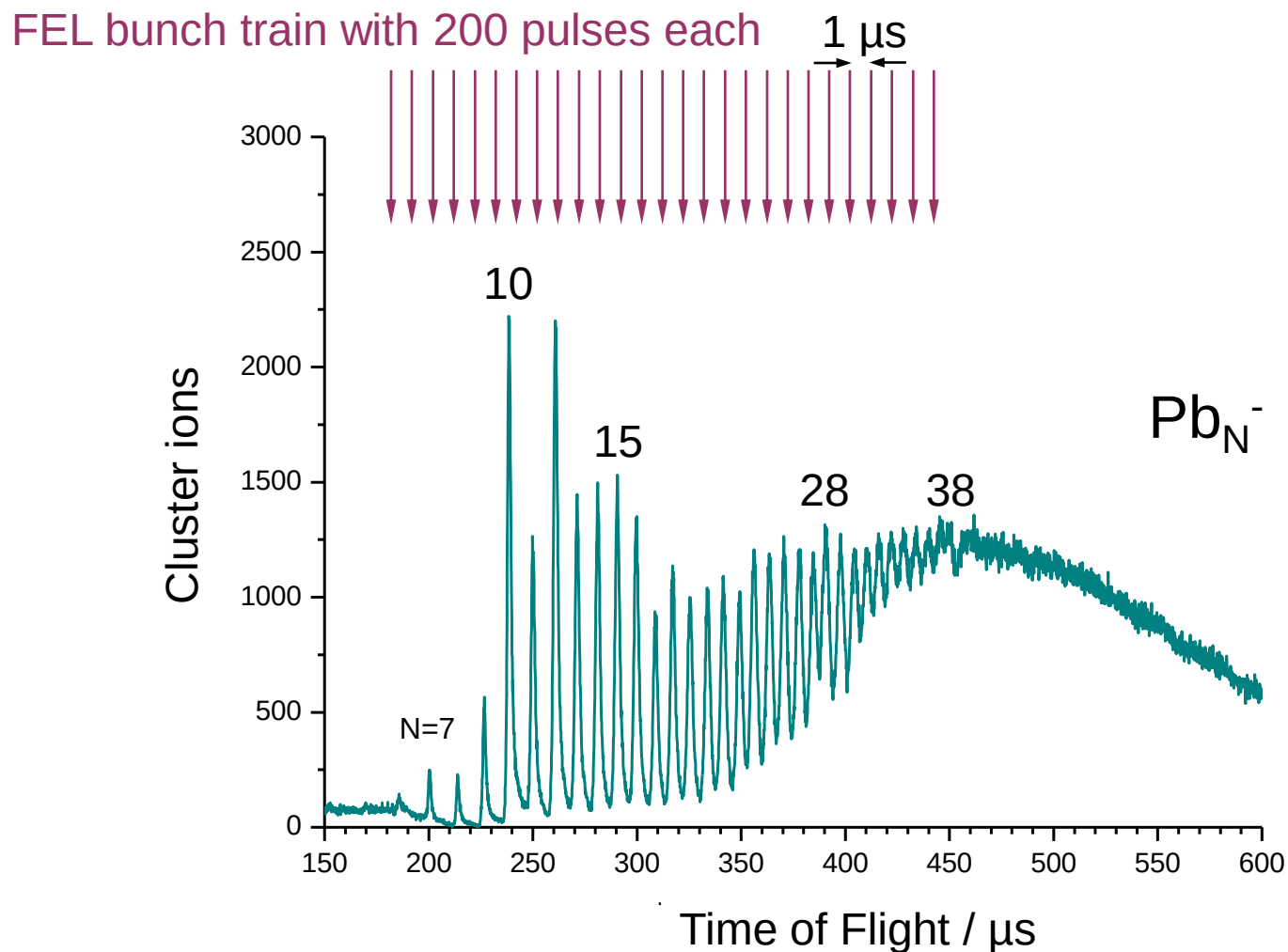
Bostedt, Fennel, Meiwes-Broer, Möller et al.,
Phys. Rev. Lett. 100:133401, 2008

**another example:
core ionization of negatively charged Pb_N**



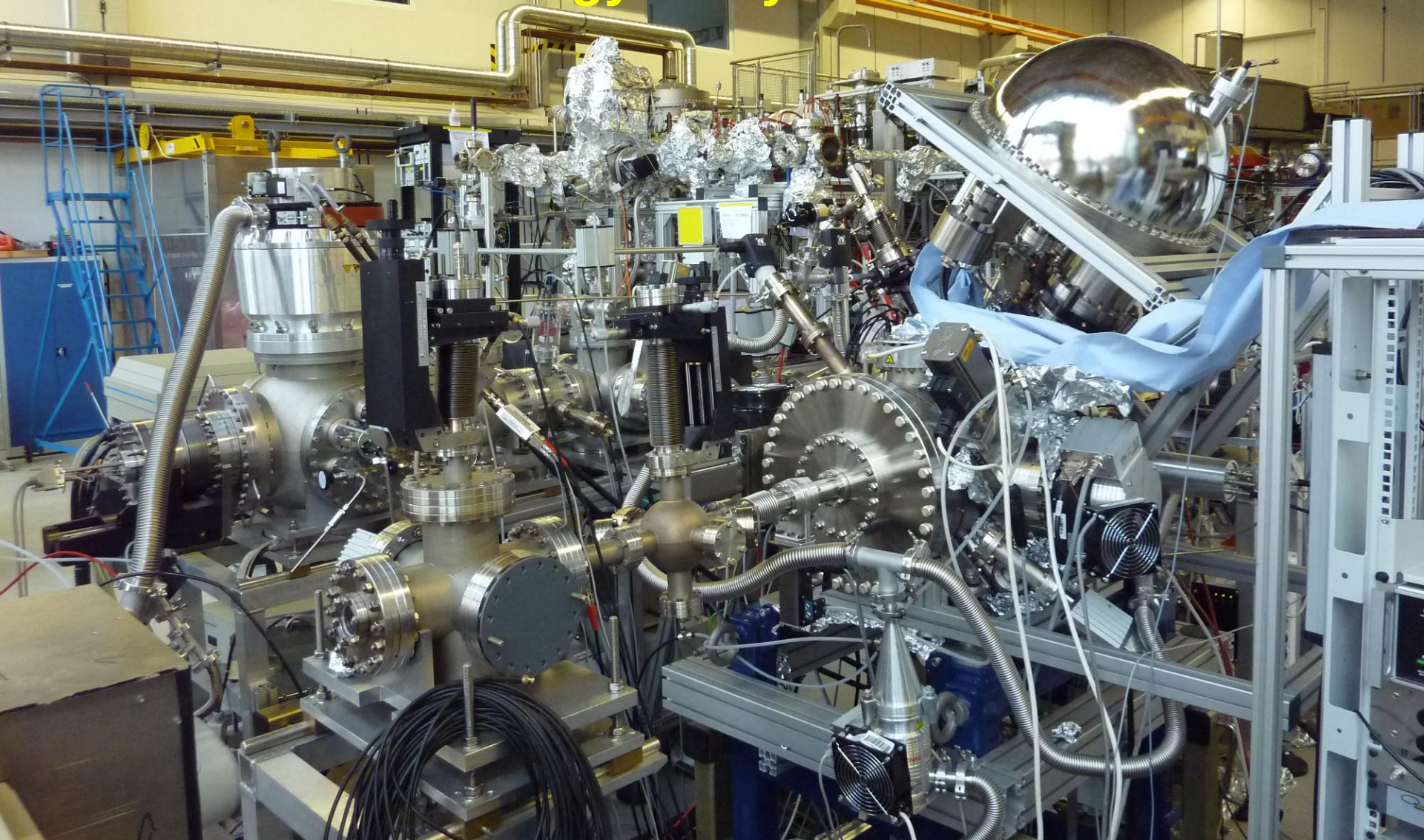
**Interesting many particle problem:
localized core hole in a *neutral* metal cluster**

using the micropulse trains of FLASH

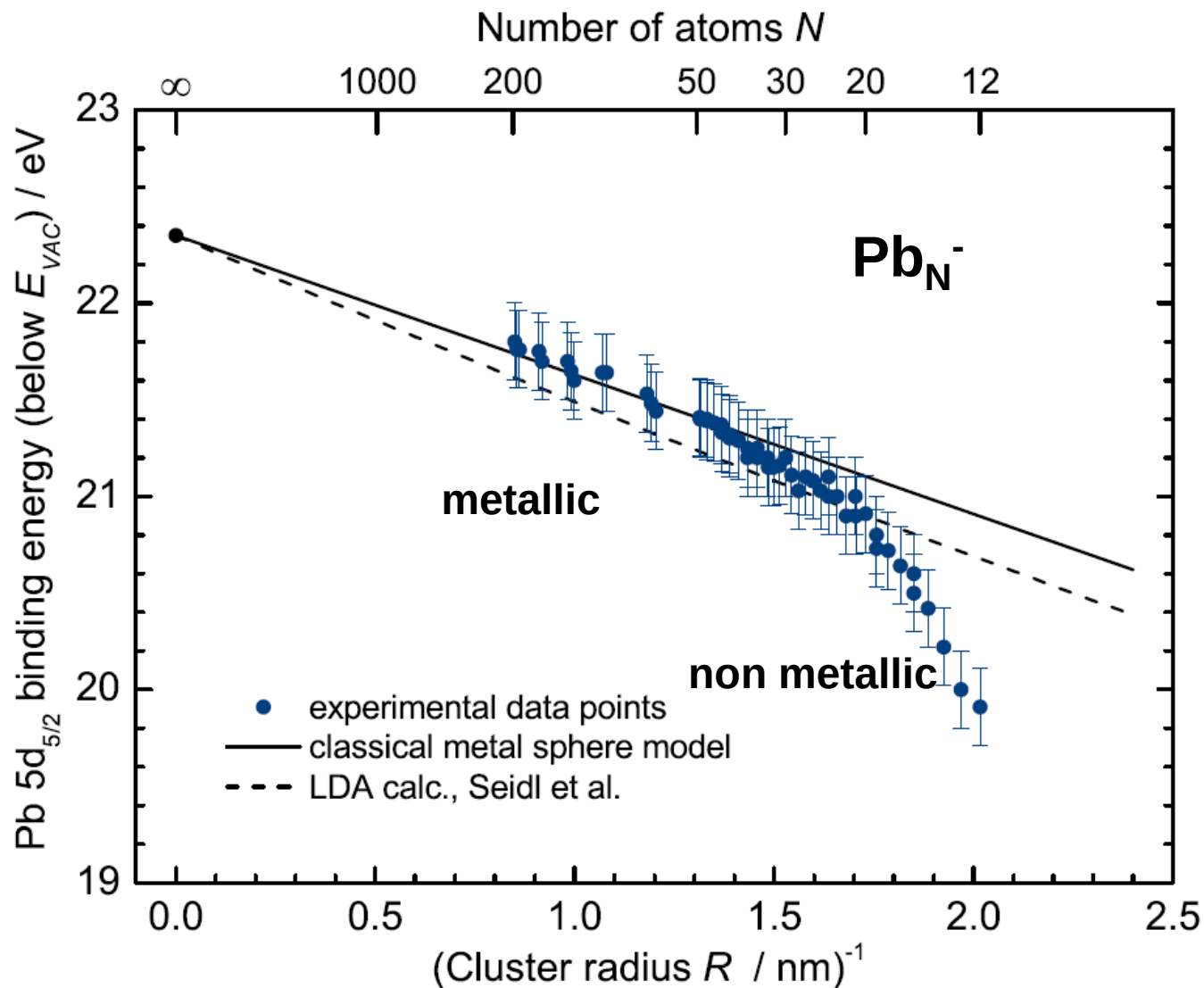


getting photoelectron spectra from each cluster size

the new hemispherical photoelectron energy analyzer



core level binding energies shift with N



Senz et al., Phys. Rev. Lett. 102 138303 (2009)



our team in Hamburg

lecture 2.12.2010

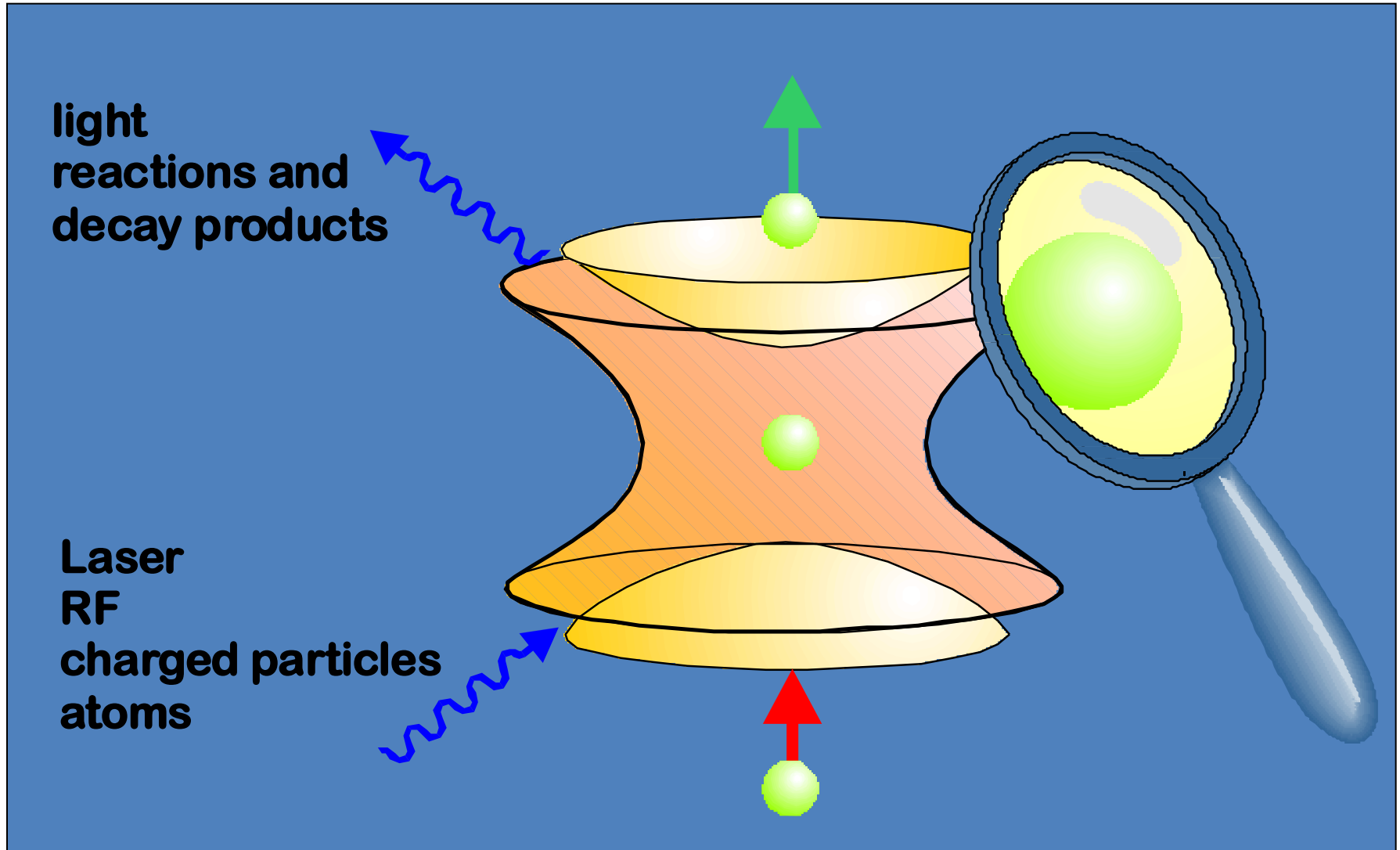
we had so far:

- Bose Einstein condensation
- trapping and cooling of ions

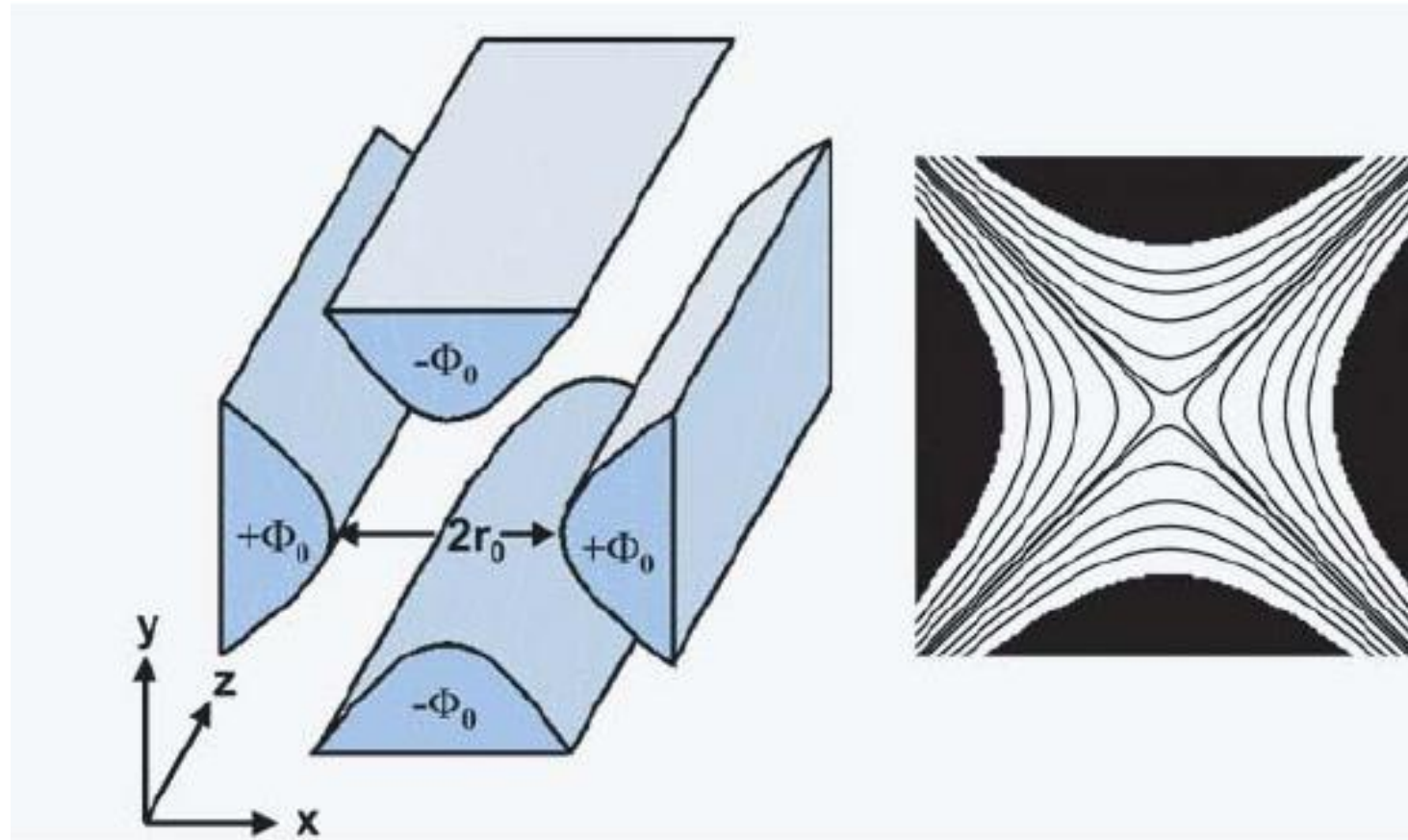
now:

- continuation with trapping and cooling of ions
- ion crystals

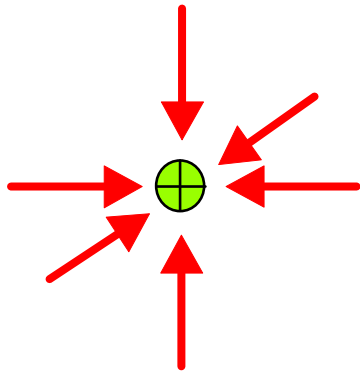
Ion traps: store, select and investigate particles in 'free' space



HF quadrupole trap in two dimensions

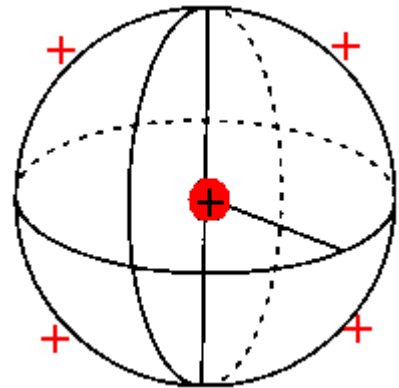


How to trap ions? Need potential minimum in 3 D

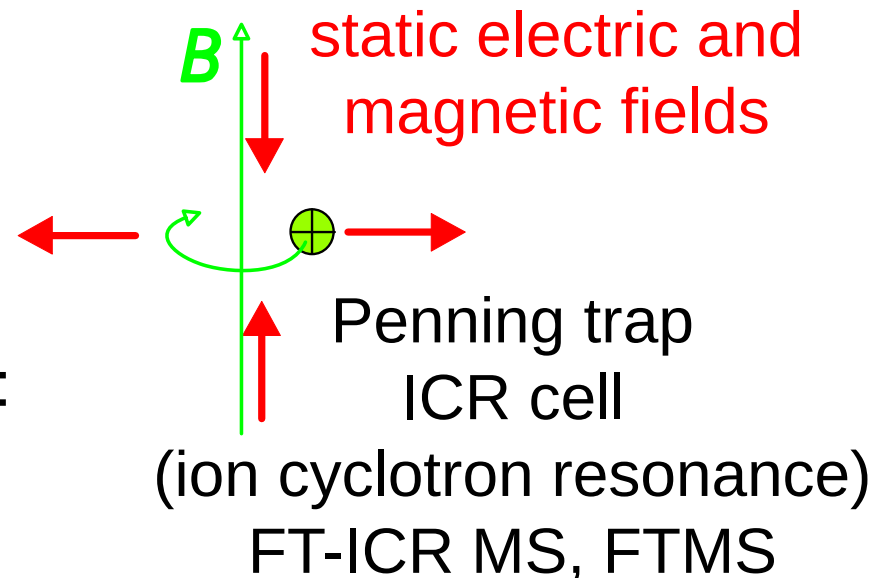
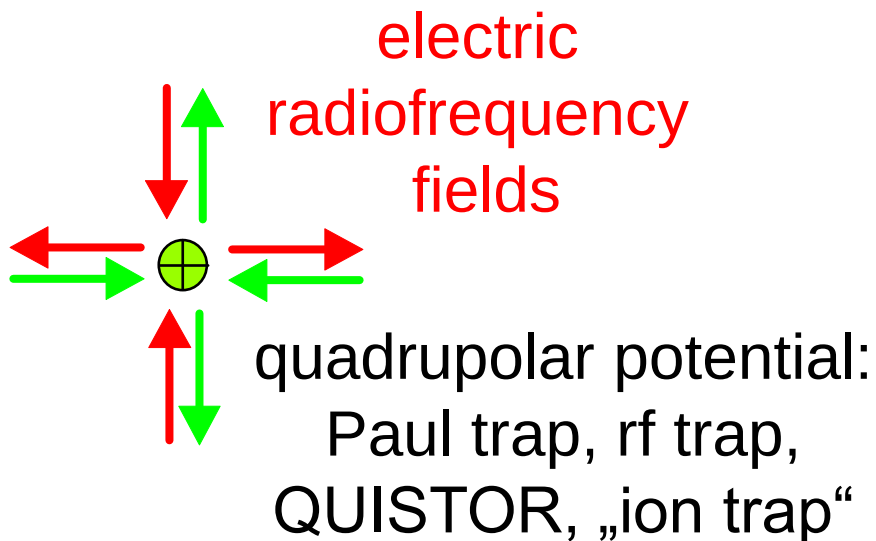


~~electrostatic trapping~~

not possible due to
Laplace: $\Delta\phi = 0$

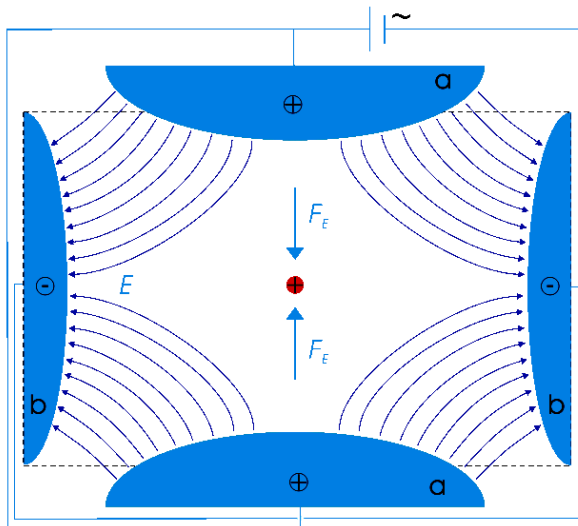


no field inside!



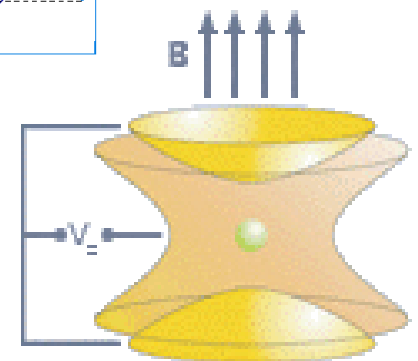
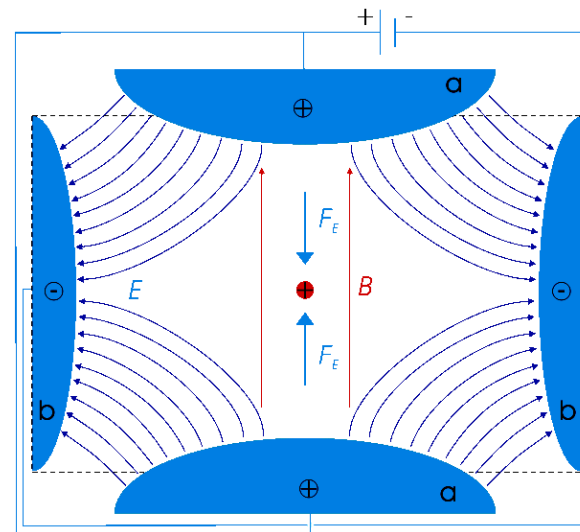
Paul trap

principle: electric
alternating field



Penning trap

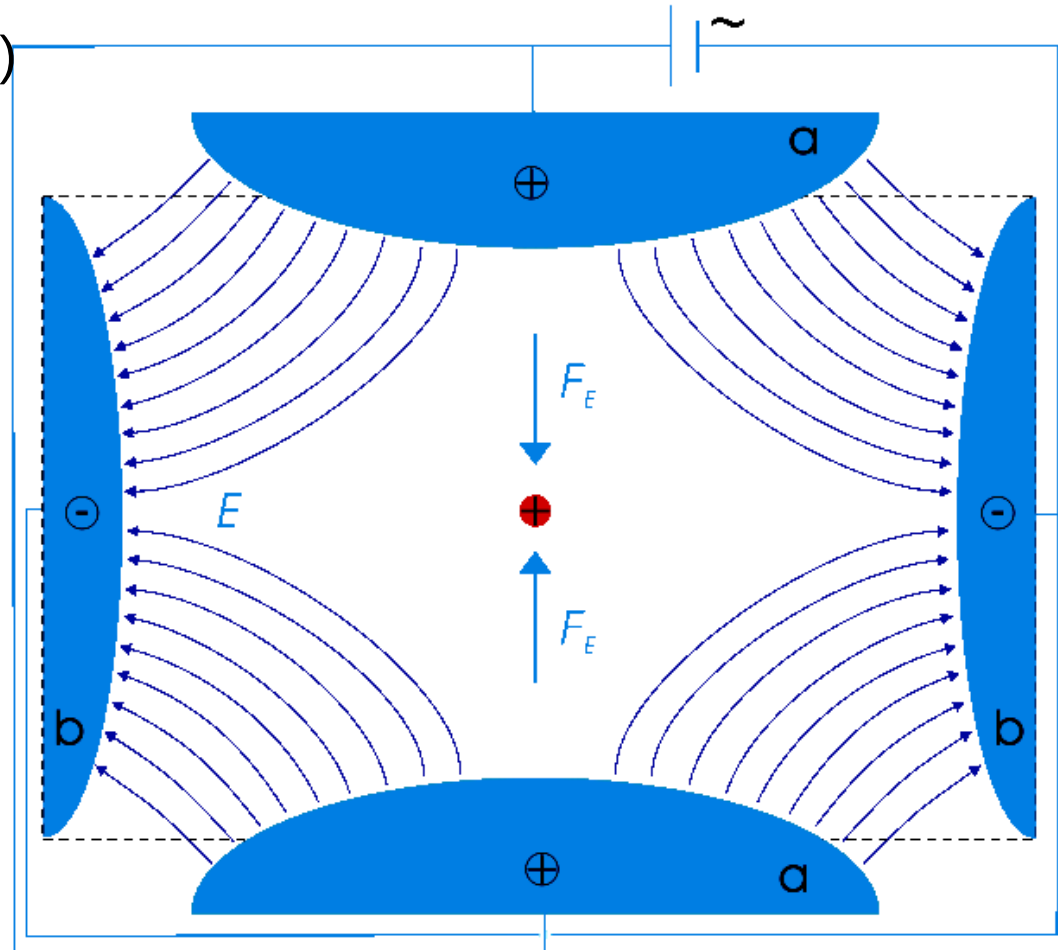
principle:
superposition of
a magnetic field



the Paul trap

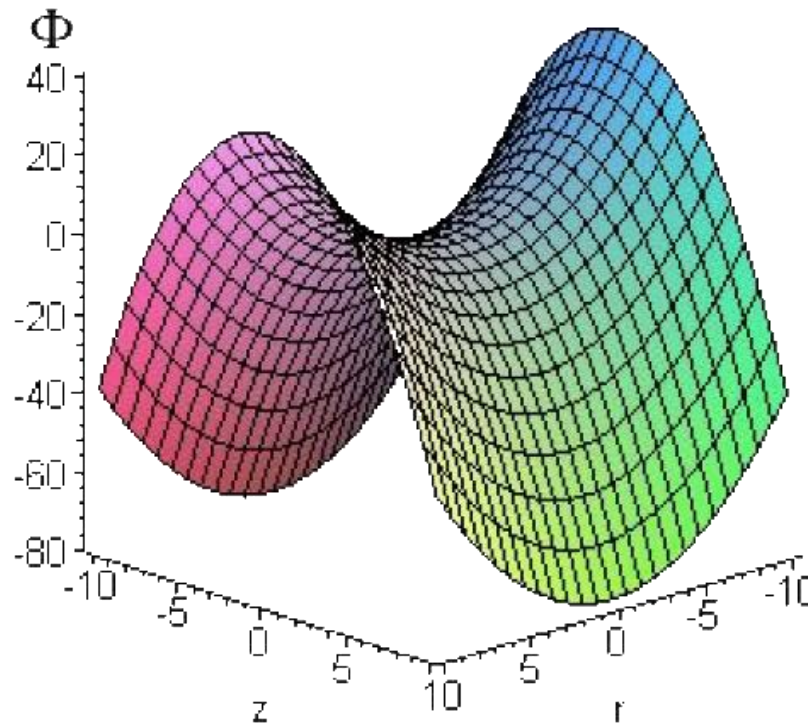
developed by
Wolfgang Paul (1913-1993)
in the 1950ies

Nobel price
in physics 1989



Electrically alternating field creates a static
pseudopotential

the potential of the Paul trap



c.f.:
the mechanical
analogon -
rotating saddle
will trap a ball

$$\Phi(x, y, z, t) = \frac{U_0 \cdot \sin \omega t}{2r_0^2} \cdot (x^2 + y^2 - 2z^2)$$

equation of motion

$$\frac{d^2 r}{dt^2} + \frac{e(U_0 + V_0 \cos(\Omega t))}{mr_0^2} r = 0 \quad \frac{d^2 z}{dt^2} - \frac{2e(U_0 + V_0 \cos(\Omega t))}{mr_0^2} z = 0$$

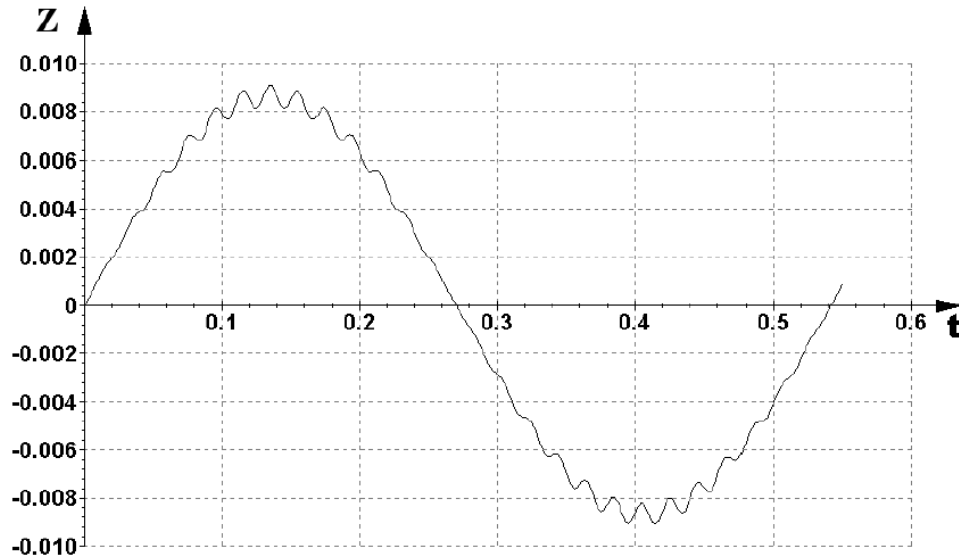
special cases of the der Mathieu- DGL

equation of motion derived from the static 'pseudo potential':

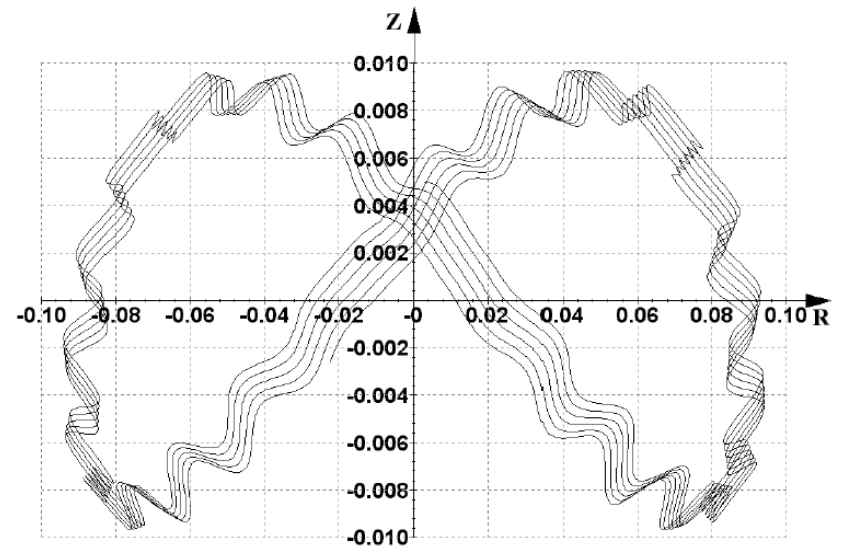
$$u(t) \propto \left[1 - \frac{q_u}{2} \cos(\Omega t) \right] \cos(\omega t - \varphi) \quad \omega = \frac{\beta_u}{2} \Omega$$

- micro motion: driven oscillation with phase locked to the exciting field
- macro motion: free oscillations of the ions in the pseudopotential

ion motion in time and space



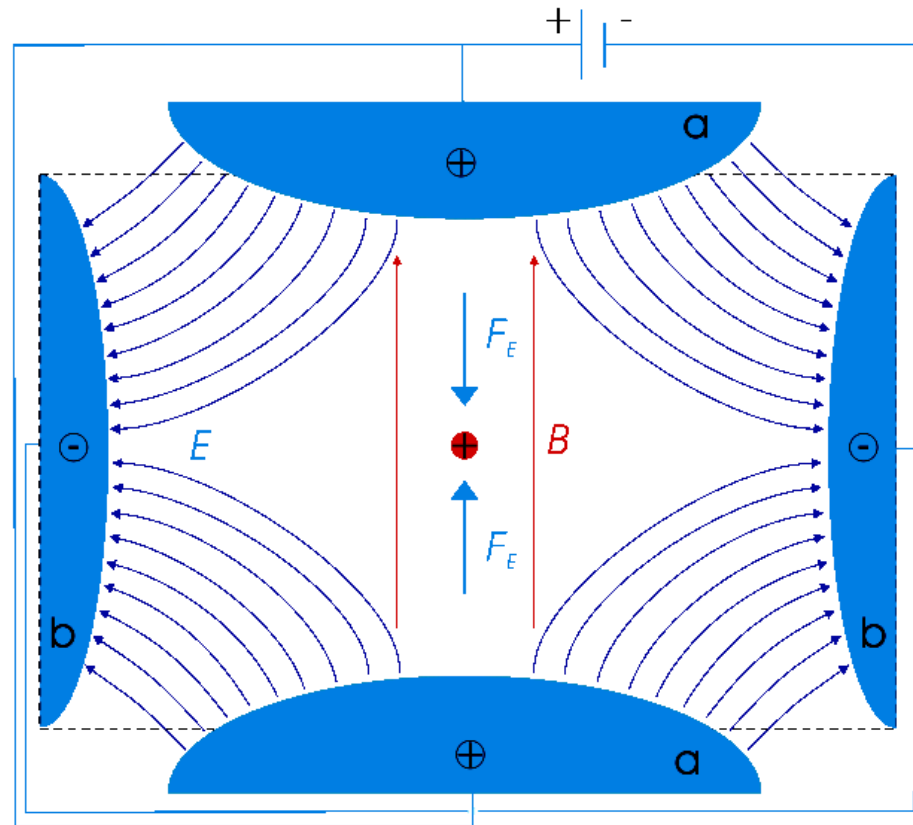
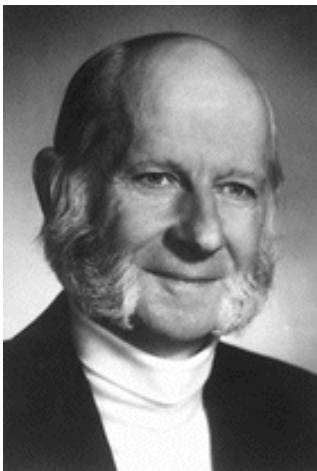
micro and macromotion



trajectory

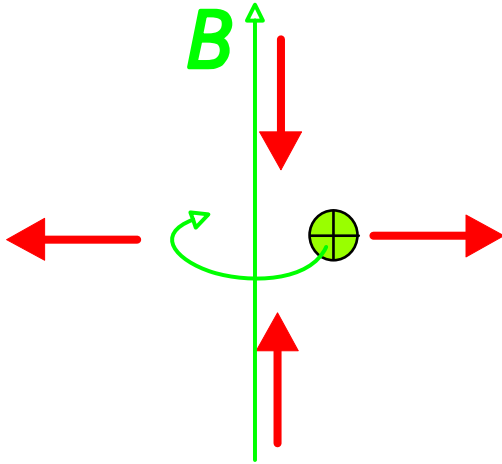
the Penning trap

idea of the Dutch Physicist Frans Michel Penning in the 1930ies



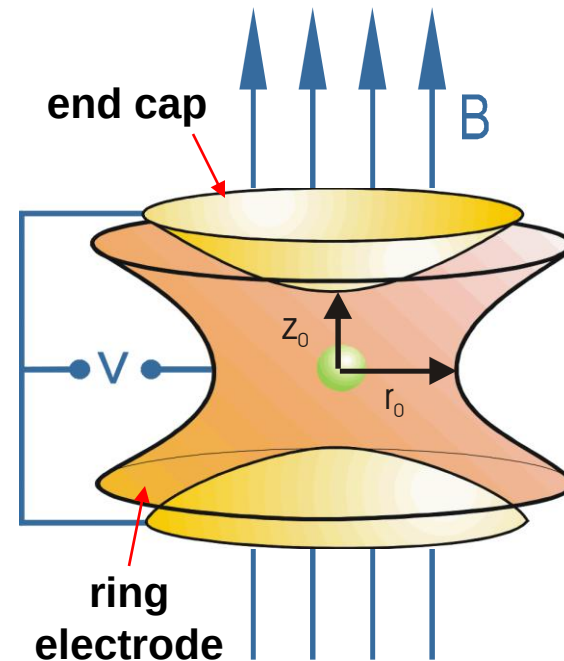
realization: Hans G. Dehmelt
(Nobel prize in physics 1989)

Principle of Penning traps (see exercise)



Cyclotron frequency:
$$f_c = \frac{1}{2\pi} \cdot \frac{q}{m} \cdot B$$

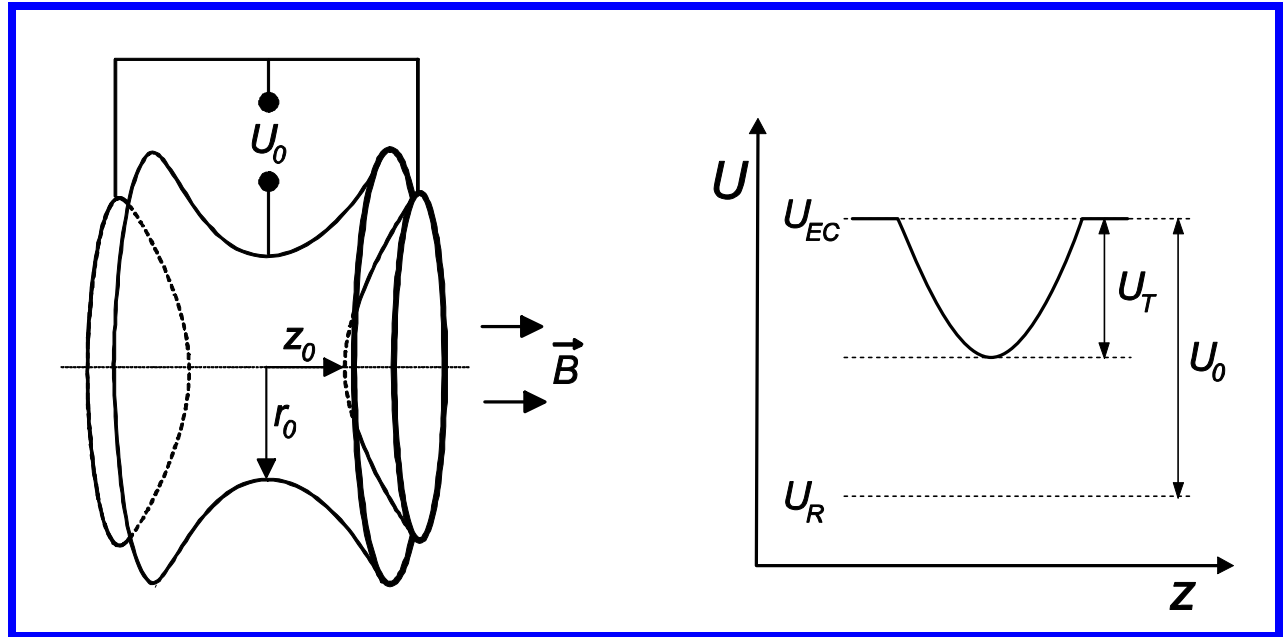
- Strong homogeneous magnetic field
- Weak electric 3D quadrupole field



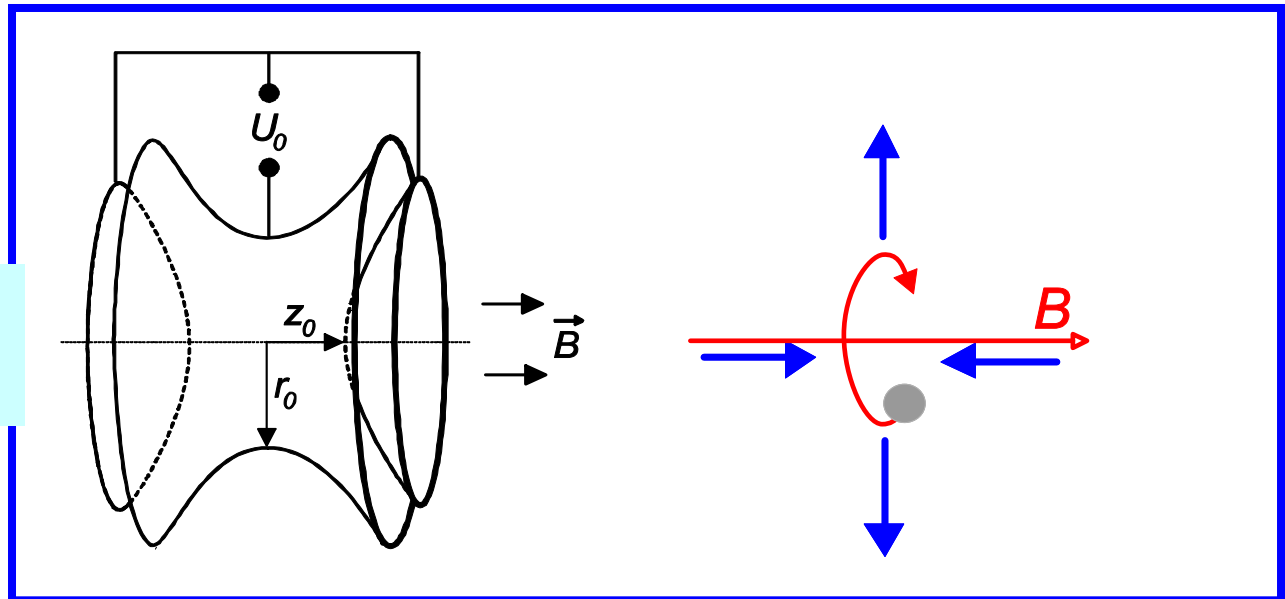
Confinement

in a Penning trap

axial harmonic
potential



radial confinement
with magnetic field



motion in the Penning trap

plus Lorentz force:

$$\vec{F} = -e_0 \vec{\nabla} \phi(r) + \vec{e}_0 v \times \vec{B}$$

equation of motion:

$$e_0(\vec{\nabla} \phi(r) + \vec{v} \times \vec{B}) + \vec{m} \ddot{\vec{r}} = 0$$

axial oscillation

$$\frac{2e_0 U_0}{m d_0^2} \cdot z + m \ddot{z} = 0$$

$$\omega_z = \sqrt{\frac{2e_0 U_0}{m d_0^2}}$$

z or axial frequency

radial oscillation

substitution:

$$u = x + iy$$

$$\omega_c = \frac{e_0}{m} B \quad i\omega_c \dot{u} - \frac{\omega_z^2}{2} u + \ddot{u} = 0$$

$$u \hookrightarrow u_0 e^{-i\omega t}$$

$$\omega_+ = \frac{\omega_c}{2} + \sqrt{\frac{\omega_c^2}{4} - \frac{\omega_z^2}{2}}$$

modified or reduced cyclotron frequency

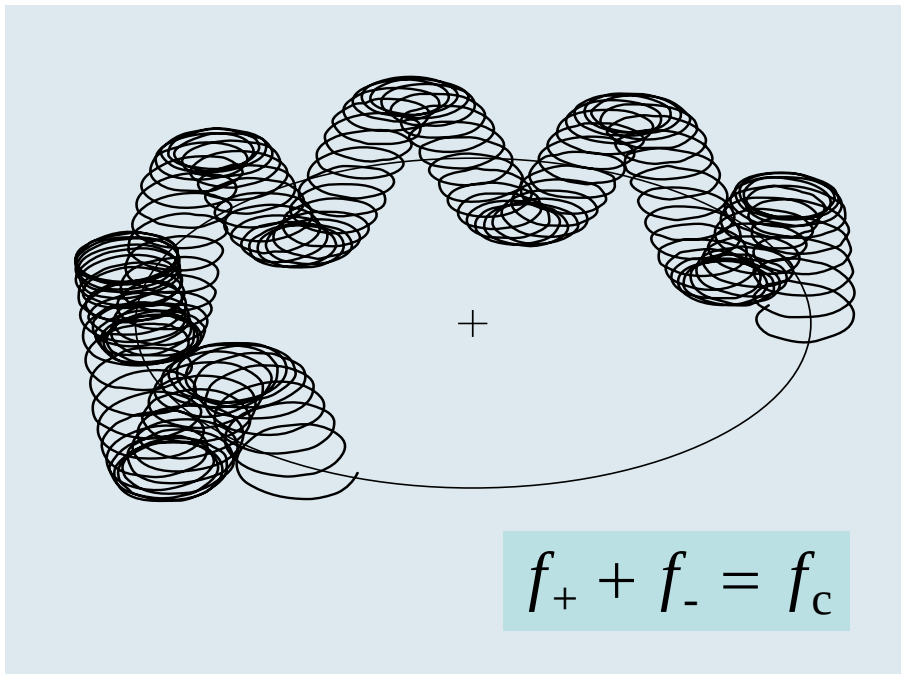
$$\omega_- = \frac{\omega_c}{2} - \sqrt{\frac{\omega_c^2}{4} - \frac{\omega_z^2}{2}}$$

magnetron frequency

Ion motion in a Penning trap

Motion of an ion is the superposition of three harmonic eigenmodes:

- axial motion (frequency f_z)
- magnetron motion (frequency f_-)
- modified cyclotron motion (frequency f_+)



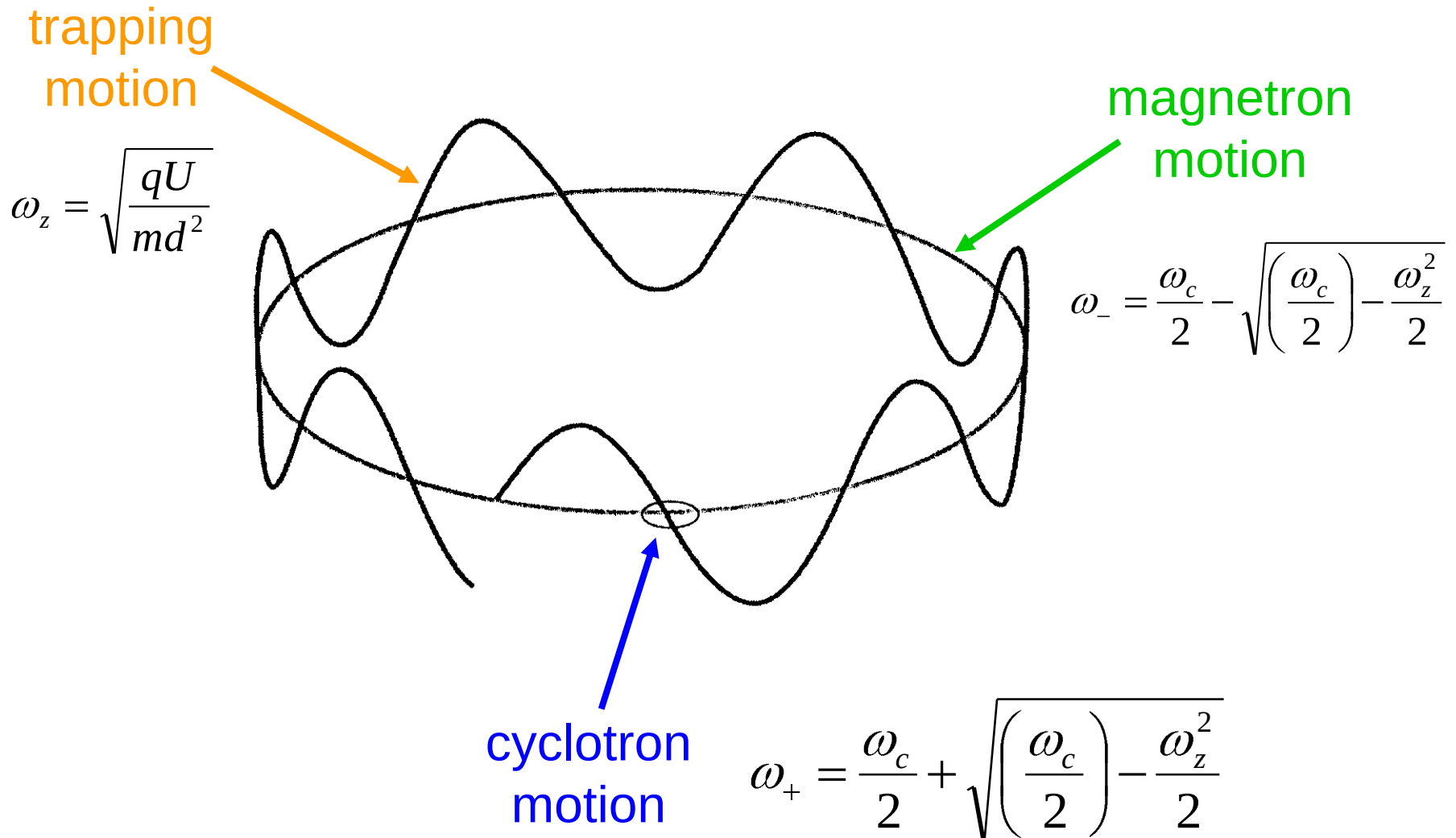
f_c := cyclotron frequency

Typical frequencies
 $q = e$, $m = 1000 \text{ u}$,
 $B = 6 \text{ T}$

$$\Rightarrow f_- \approx 1 \text{ kHz}$$
$$f_+ \approx 100 \text{ kHz}$$

L.S. Brown, G. Gabrielse,
Rev. Mod. Phys. 58, 233 (1986).

another view on the ion motion in Penning trap

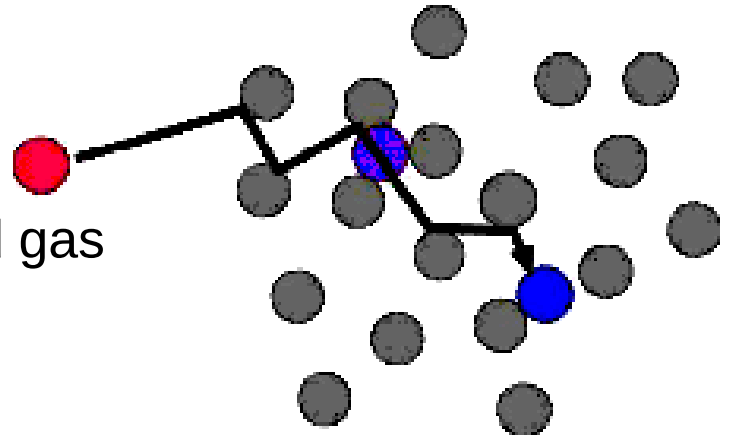


cooling methods

- buffer gas collisions
- electron collisions
- evaporation cooling
- Laser cooling
- sympathetic cooling

buffer gas cooling:

- collisions with a cold gas
- final temperature is temp. of the cold gas
- good for all particles

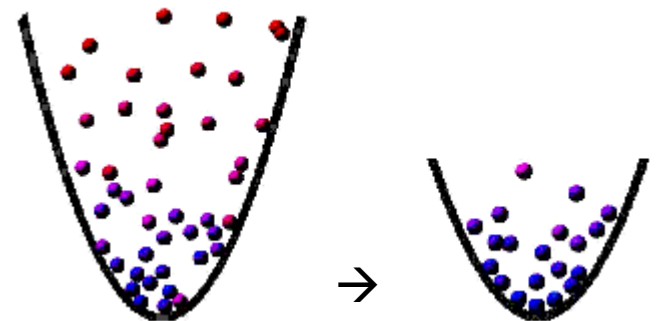


electron collisions cooling:

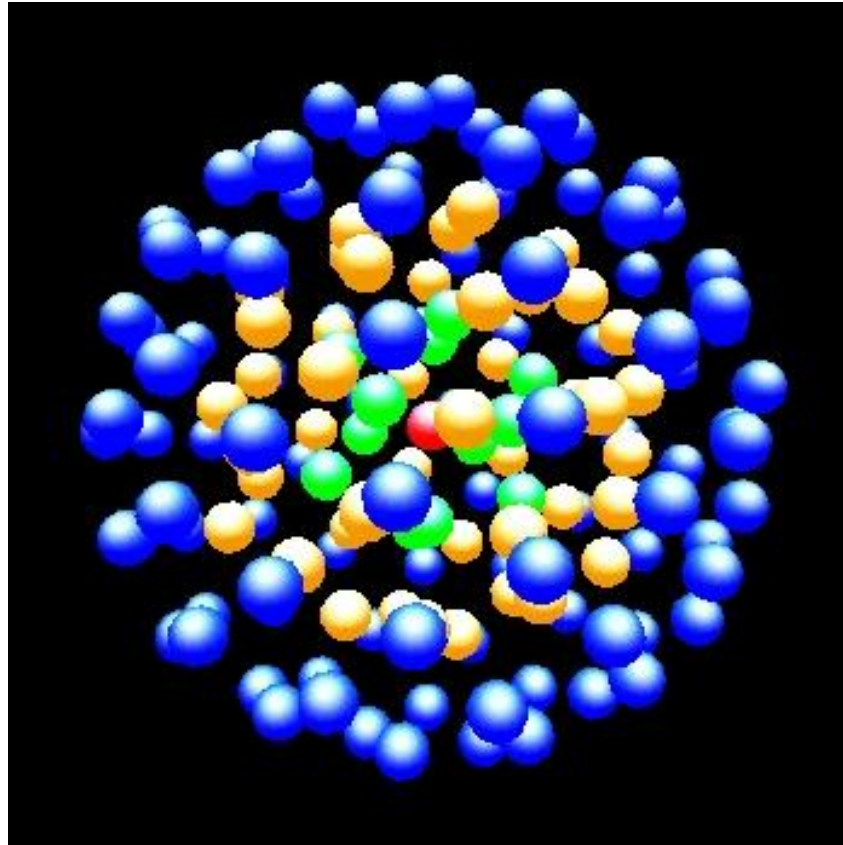
- co-propagating electron beam
 - ion velocity ultimately adapts the electron velocity
- monoenergetic ion beam with low divergence

evaporation cooling:

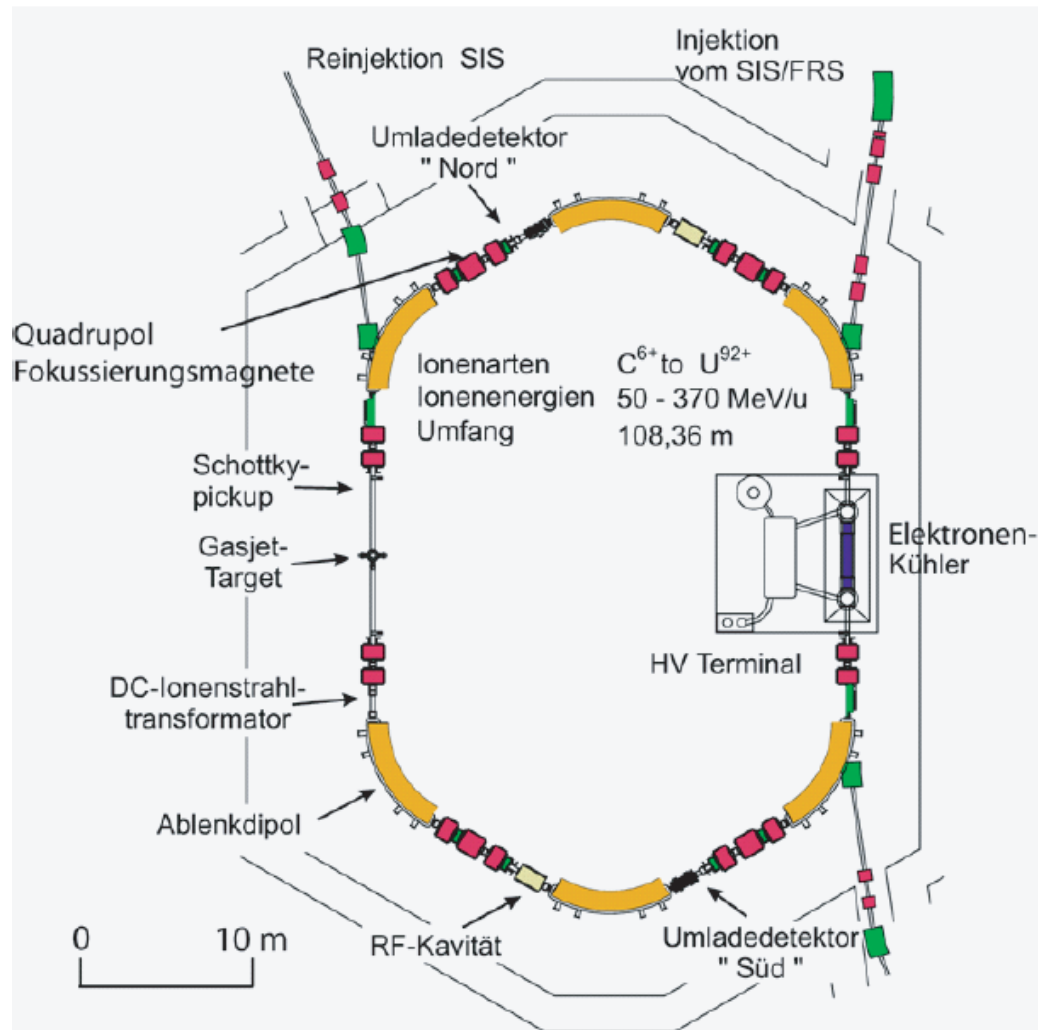
- hot atoms of the **Maxwell-Boltzmann distribution** will be removed



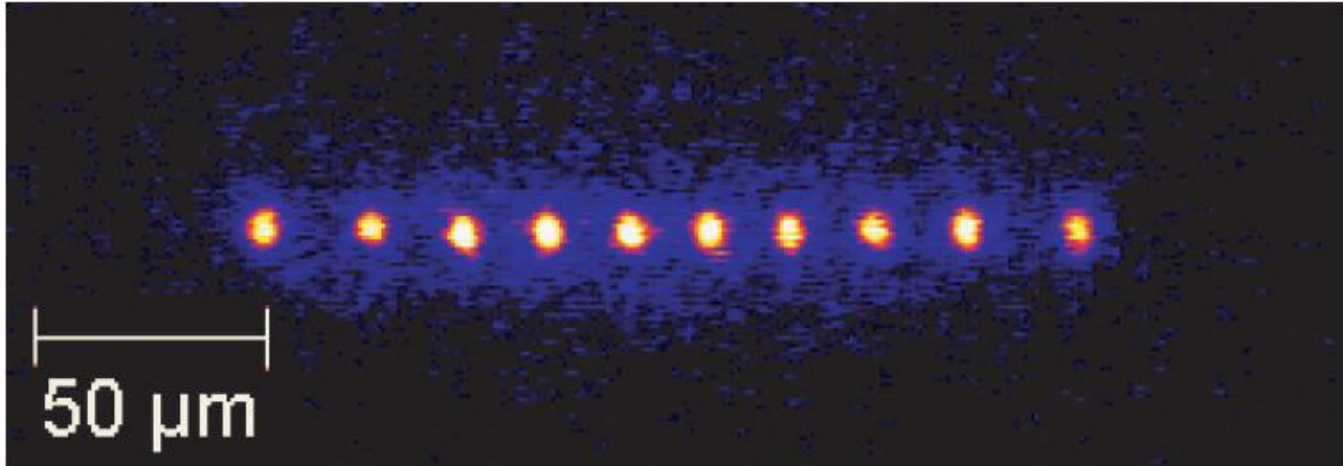
Wigner crystal



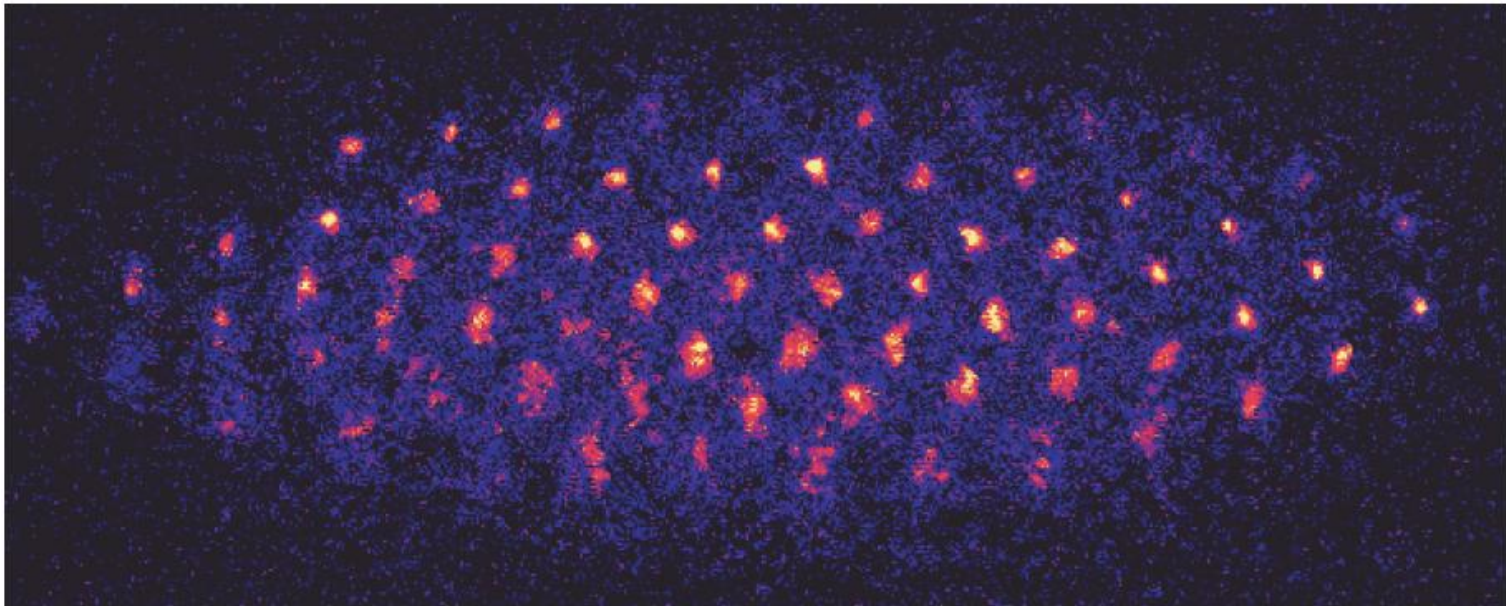
storage ring at the GSI Darmstadt



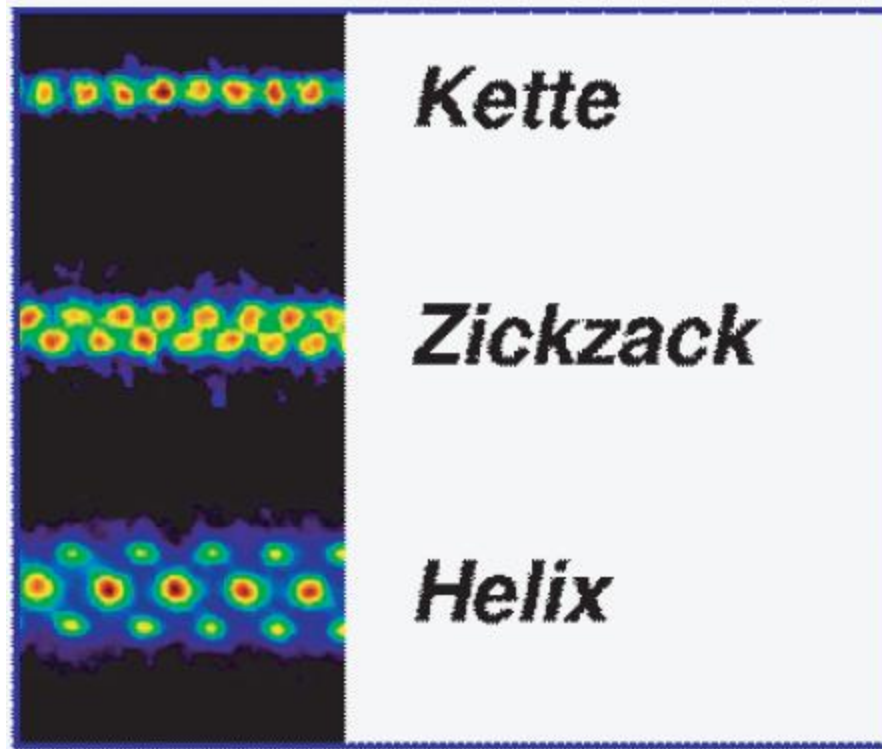
Calcium ions in a linear Paul trap



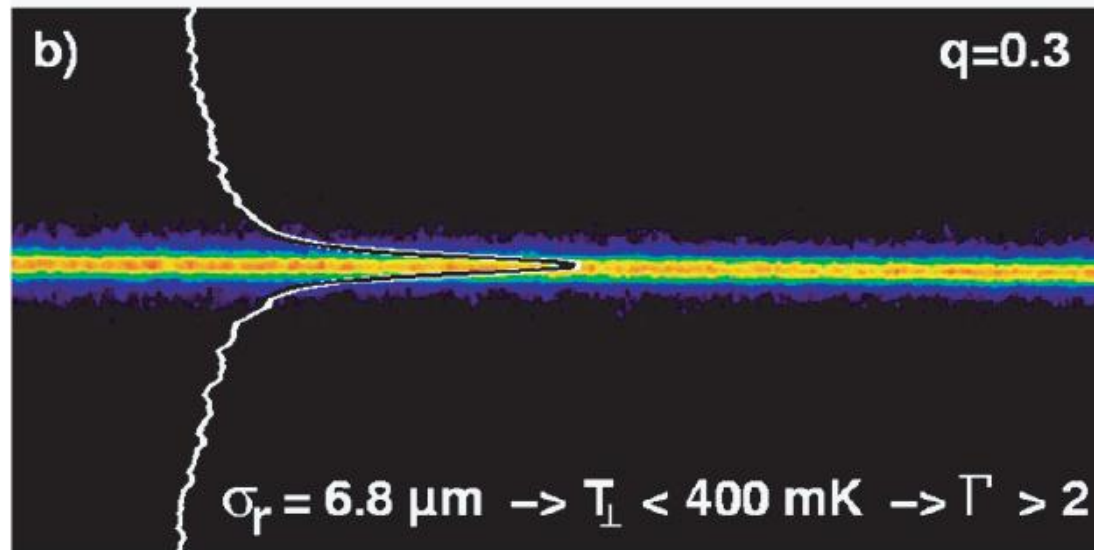
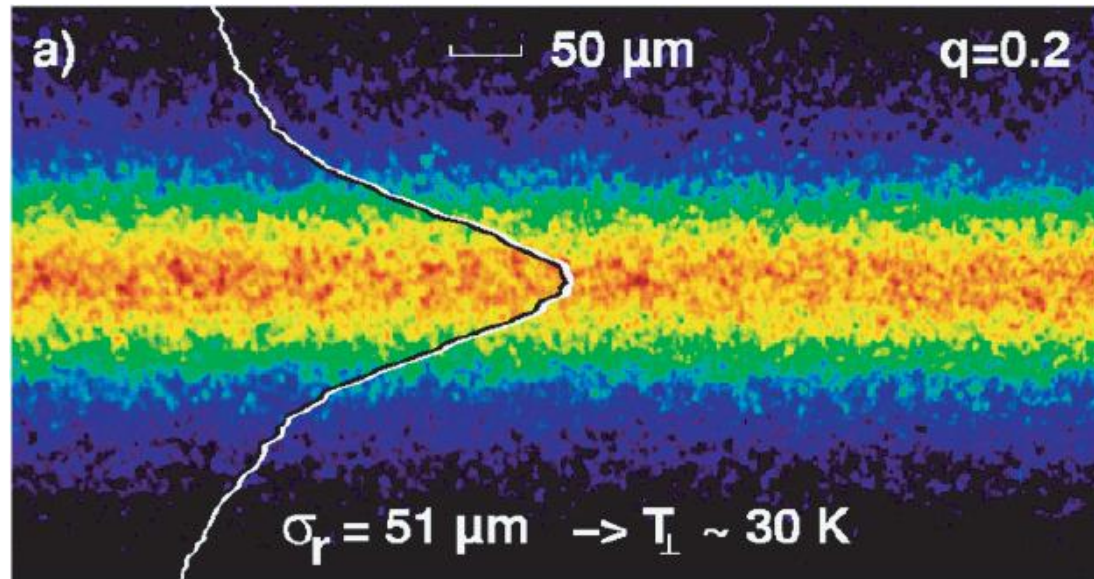
Calcium ions crystal



ion crystals at different linear densities

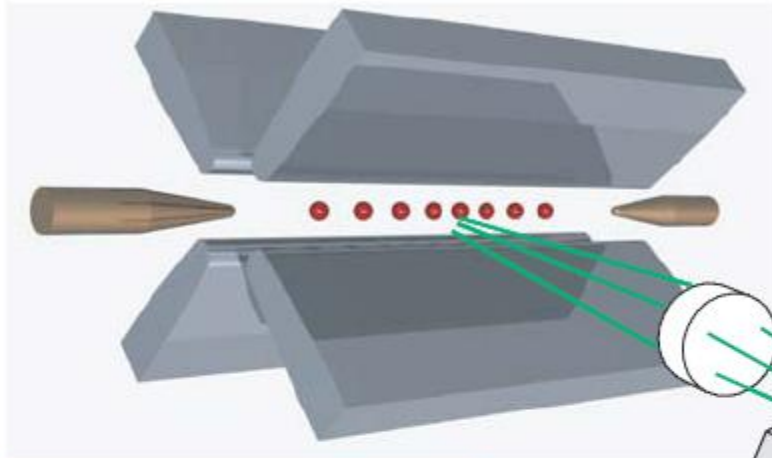


phase transition from liquid to crystalline phase in an ion beam



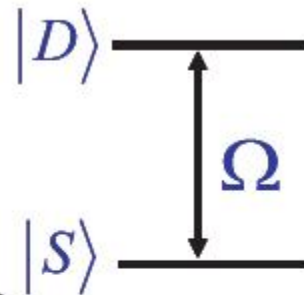
ions can be crystallized and manipulated for quantum information

$^{40}\text{Ca}^+$ -Ionenkette in einer Paul-Falle

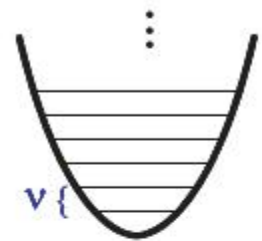


Ionen-Qubits bilden ein Quantenregister

2-Niveau-Atom



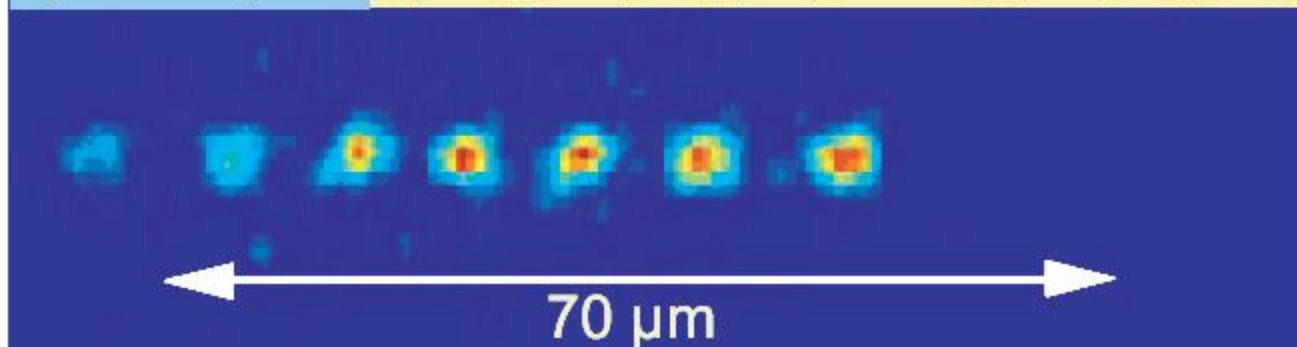
harm. Falle



Quantenbit (Qubit)

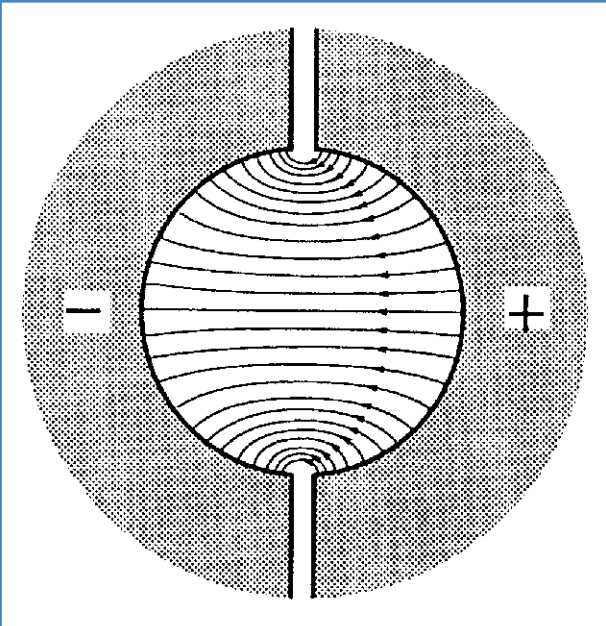
$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle$$

Quantenregister $|\psi\rangle = c_{000}|000\rangle + c_{001}|001\rangle + \dots + c_{110}|110\rangle + c_{111}|111\rangle$

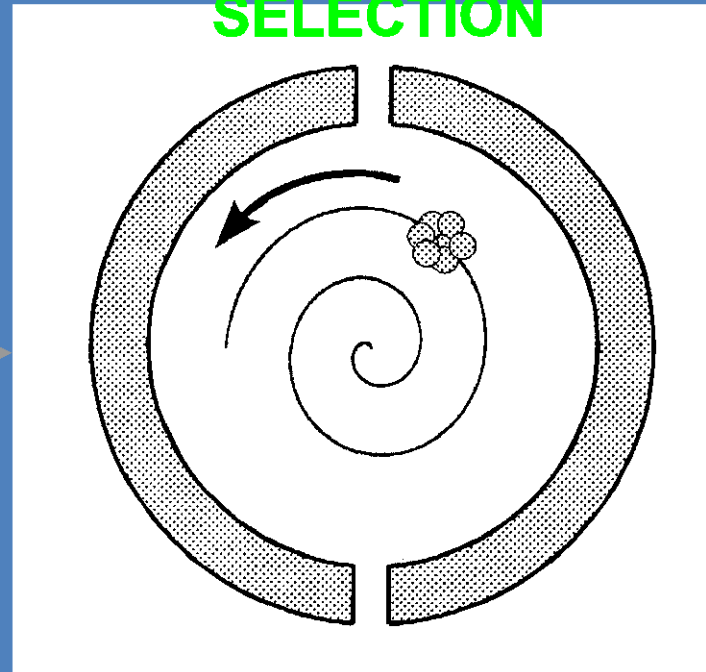


manipulation of ion motion in a penning trap for mass spectroscopy

DIPOLAR EXCITATION

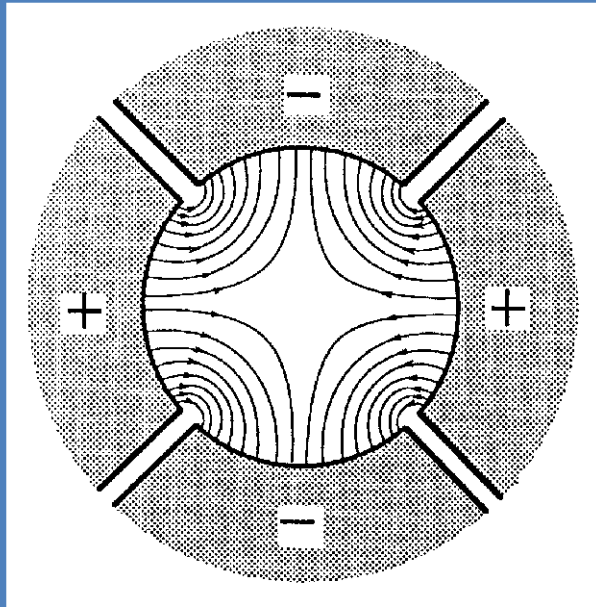


**KINETIC ENERGY
AND
SELECTION**



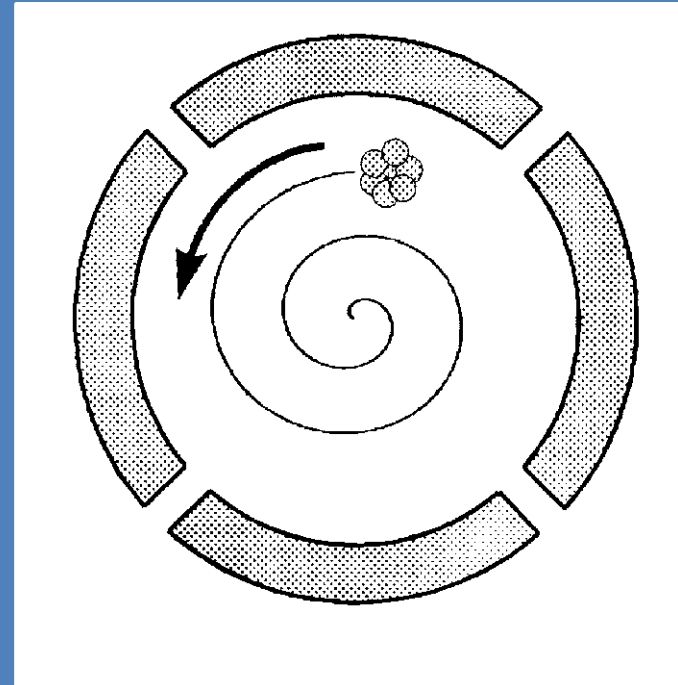
Manipulation of ion motion

QUADRUPOLEAR EXCITATION (BUFFER GAS ASSISTED)



CENTERING

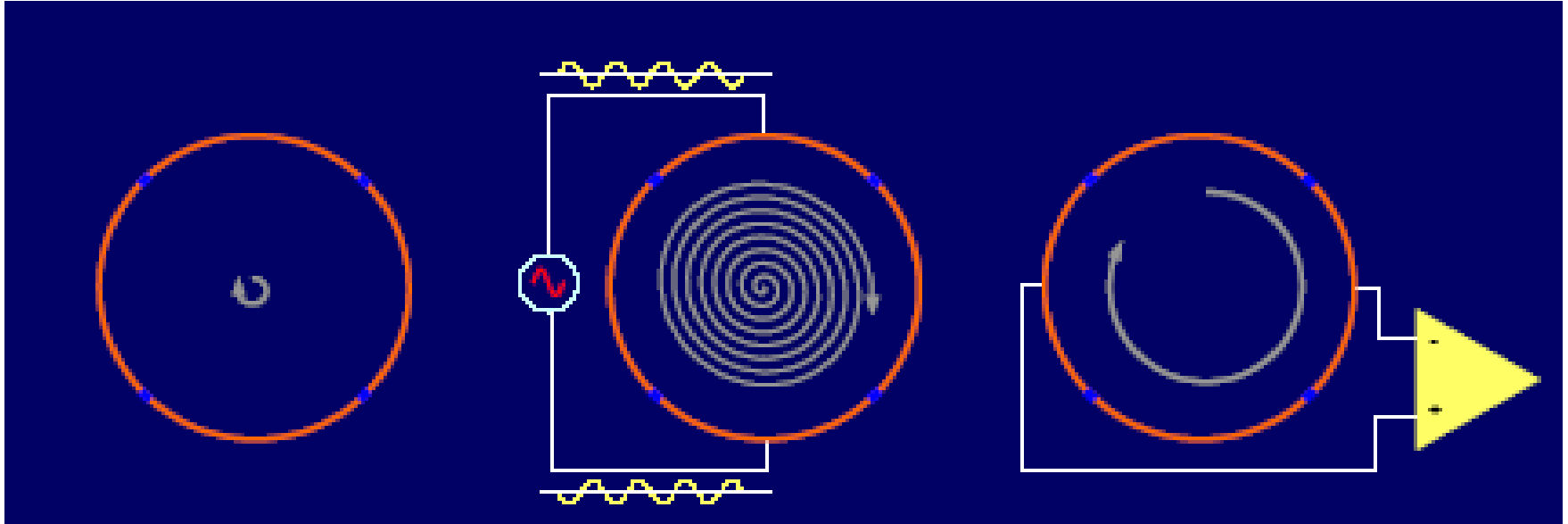
Savard et al., Phys. Lett A, 1991



„Axialization“

L.S. et al., IJMS (1992)

Fourier transform ion cyclotron resonance mass spectroscopy FTICR

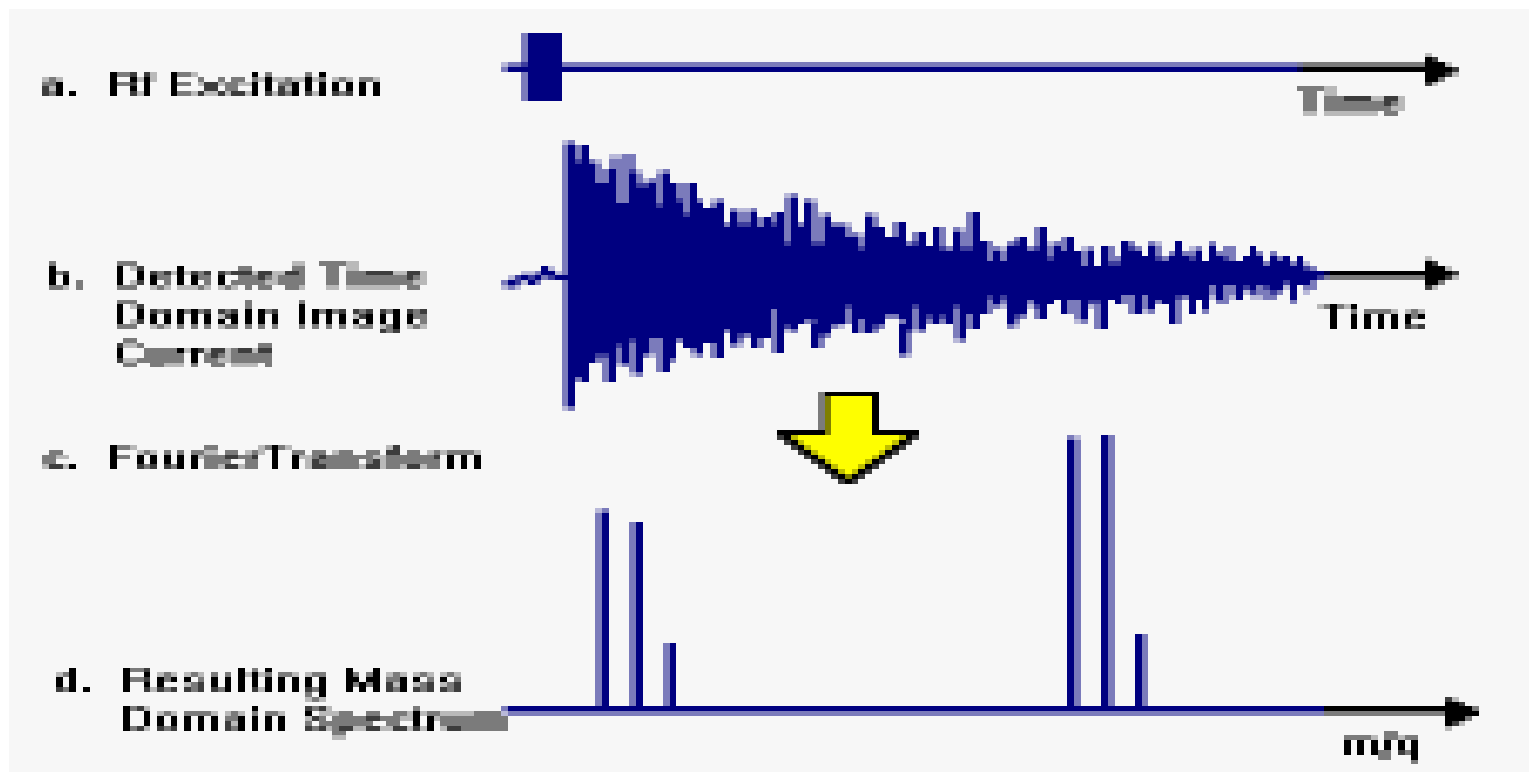


- Ions are trapped and oscillate with low, incoherent, thermal amplitude
- Excitation sweeps resonant ions into a large, coherent cyclotron orbit
- Preamplifier and digitizer pick up the induced potentials on the cell wall

FTICR

Image is Fourier transformed to obtain the component frequencies and amplitudes (intensity) of the various ions.

Cyclotron frequency value is converted into a m/z value to produce mass spectrum with the appropriate intensities.





Thermo Finnigan FT ICR
(Ion cyclotron resonance)
11.5 Tesla
Massenspektrometer

FTICR

High mass resolution $> 3\,000\,000$

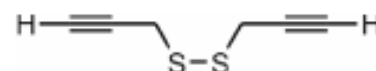
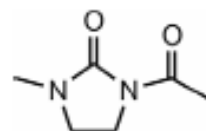
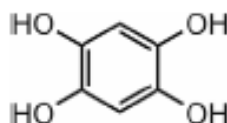
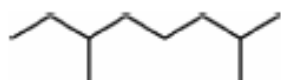
Accuracy of mass determination $< 0.1\text{ ppm}$

Sensitivity (ESI, Octapeptide) ca. 50 attomol

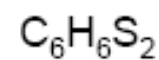
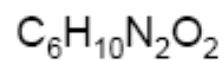
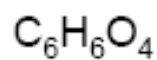
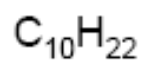
Structure-specific fragmentation MS/MS , MSⁿ

Exact Masses and Molecular Formulae

So, molecules with different molecular formulae have different exact masses.



molecular
formula



m/z
(unit)

142

142

142

142

m/z
(exact mass)

142.1723

142.0264

142.0743

141.9911

<i>Element</i>	<i>Atomic Weight</i>	<i>Nuclide</i>	<i>Mass</i>	<i>Relative Abundance</i>
Hydrogen	1.00797	^1H	1.00783	100.0
		D(^2H)	2.01410	0.015
Carbon	12.01115	^{12}C	12.00000 ^b	100.0
		^{13}C	13.00336	1.11
Nitrogen	14.0067	^{14}N	14.0031	100.0
		^{15}N	15.0001	0.37
Oxygen	15.9994	^{16}O	15.9949	100.0
		^{17}O	16.9991	0.04
		^{18}O	17.9992	0.20
Fluorine	18.9984	^{19}F	18.9984	100.0
Silicon	28.086	^{28}Si	27.9769	100.0
		^{29}Si	28.9765	5.06
		^{30}Si	29.9738	3.36
Phosphorus	30.974	^{31}P	30.9738	100.0
Sulfur	32.064	^{32}S	31.9721	100.0
		^{33}S	32.9715	0.79
		^{34}S	33.9679	4.43

^{12}C mass set to
12 amu,
exactly.

As a result,
 ^1H mass is
actually higher
than 1 amu.

And ^{16}O mass is
lower than 16
amu.

Isotopes vary from unit masses by “mass defect”.

^1H has positive mass defect; ^{16}O has negative mass defect.

FTMS Extreme Resolution

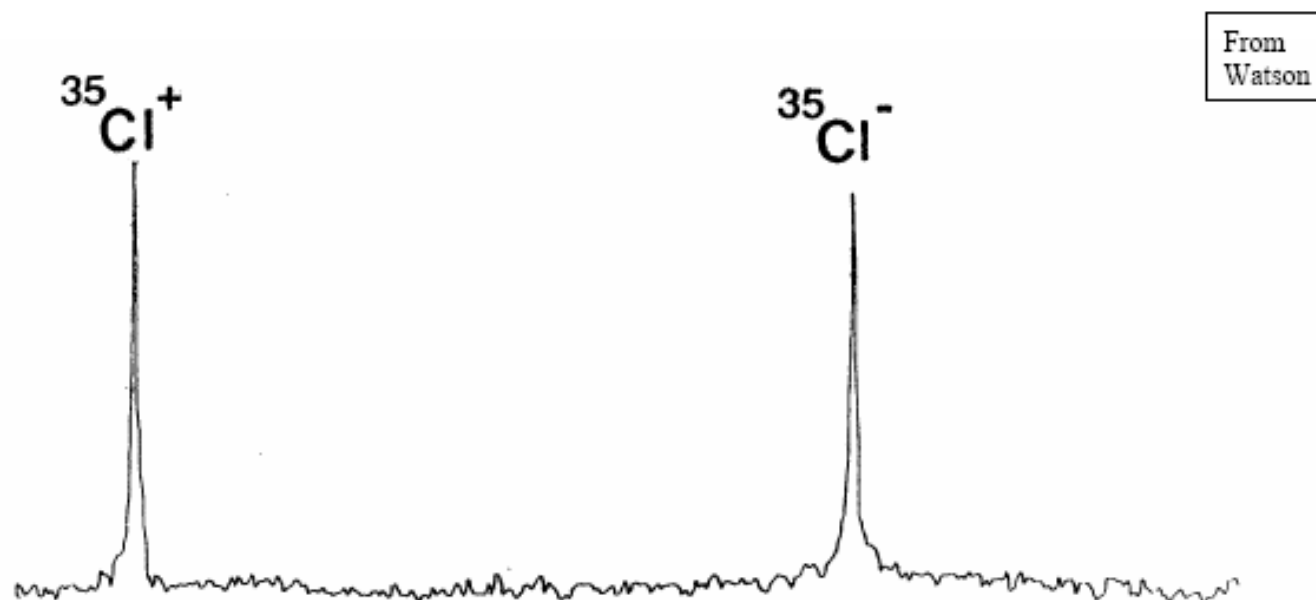
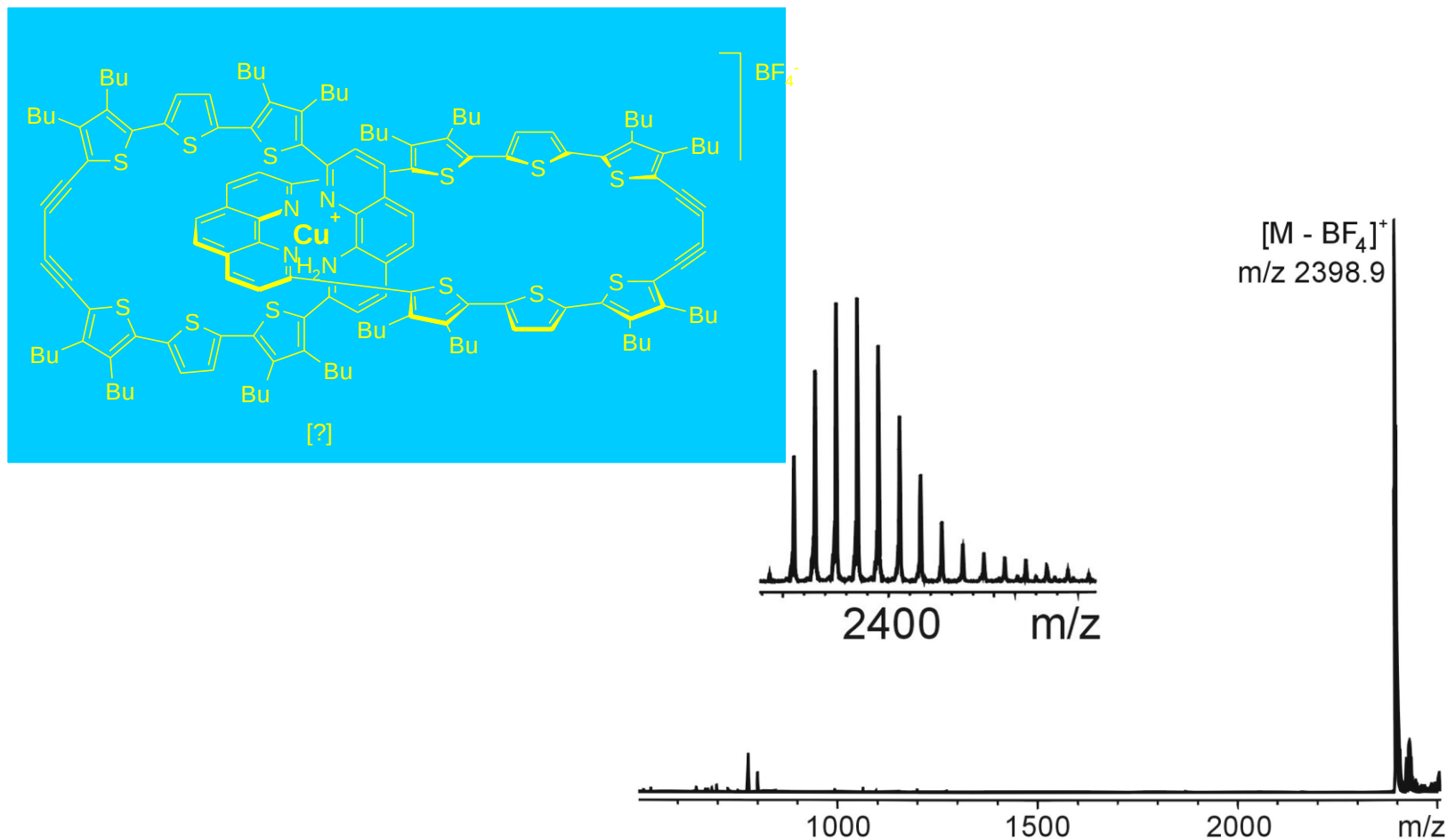


FIG. 4.22. Segment of mass spectrum in region of nominal mass 35 showing a resolution greater than 1,000,000 (FWHM definition) when using FT-MS. The peaks represent the positive and negative ions of ^{35}Cl that have a difference in mass equivalent to the mass of two electrons. The spectrum was obtained using a FT-ICR mass spectrometer with a superconducting magnet (4.7 tesla); the instrument was switched from the positive-ion-detection mode to the negative-ion-detection mode during the scan between the two peaks (Courtesy of Spectrospin AG.)

FTICR: New Dimensions of High Performance Mass Spectrometry



trapped antihydrogen

Nature October 2010

