



Paul traps

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Physics with Trapped Charged Particles, Les Houches/F







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Physics with Trapped Charged Particles, Les Houches/F

- A. Paul's work on ion traps
 - 1. Wolfgang Paul
 - 2. An ion cage
 - 3. Nobel prize
 - 4. The quadrupole ion trap
- B. Basic operation of Paul trap (single ion, no interaction)
 - 1. Mathieu equations, stability diagram
 - 2. Motion of the ion in the trap
 - 3. The adiabatic approximation
- C. Lamb-Dicke regime
 - 1. for microwaves; for optics
 - 2. how to reach LD, micromotion issues
 - 3. how to reduce micromotion; different techniques
- D. More than one ion
 - 1. space charge effects
- E. Characterisation of trap
 - 1. nonlinear resonances and canyons
 - 2. experimentally: how do I measure frequencies of motion of the trapped ions
 - 1. by fluorescence, or other optical means
 - 2. electronically (tickle, image currents;;)

- F. Modified geometries
 - 1. how, why, for what
 - 2. linear traps
 - 3. more exotic forms: the race track, the ion circus
 - 4. linear multipoles
 - 5. 2D, 3D and surface traps
 - 6. other geometries, school experiments demonstration
- G. Microfabricated traps and heating
- H. How to set up a Paul trap,
 - 1. experimental set-up; rf drive, helical resonator, how to p the drive +-V0 or +-V/2
 - 2. how to detect ions in the trap
 - 1. by construction (die glaserne Paulfalle, with inegr fibers, stylus ion trap)
 - 2. by optical means
 - 3. by electronic means
- I. Tutorial: how to design an ion trap?





« Mich dünkt , es ist ein trauriger Umstand bei unserer ganzen Chemie, dass wir die Bestandteile der Körper nicht frei suspendieren können »

« I believe, it is a sad fact in all our chemistry, that we are not able to freely suspend the elementary constituents »

Georg Christoph Lichtenberg (1742-1799)



A. Paul's work on ion traps



Wolfgang Paul

- 1913 1983
- was an expert in mass filters
- since 1952, professor at University Bonn
- responsibilities at KFA Jülich, CERN (director of Nuclear Physics Division), DESY
- intended to work on « strong focussing » for a 500 MeV synchrotron
- the ion trap was a by-product of the mass selection efforts



A. Paul's work on ion traps

FORSCHUNGSBERICHTE DES WIRTSCHAFTS- UND VERKEHRSMINISTERIUMS NORDRHEIN-WESTFALEN

Herausgegeben von Staatssekretär Prof. Dr. h. c. Dr. E. h. Leo Brandt

Nr. 415

Prof. Dr.-Ing. Wolfgang Paul Dr. rer. nat. Otto Osberghaus Dipl.-Phys. Erhardt Fischer Physikalisches Institut der Universität Bonn

Ein Ionenkäfig

1958

« An ion cage »

Martina Knoop – Jan 2018







The Nobel Prize in Physics 1989

The Royal Swedish Academy of Sciences has a warded this year's Nobel Prize in Physics for contributions of importance for the development of atomic precision spectroscopy



Hans Dehmelt University of Washington Seattle, USA **Wolf gang Paul** Universität Bonn Federal Republic of Germany

for the development of the ion trap technique Norman F. Ramsey Harvard University Cambridge, USA

for the invention of the separated oscillatory fields method and its use in the hydrogen maser and other atomic clocks

A. The ion cage







B. Operation of Paul trap



 a ring and 2 endcaps of hyperboloid shape

- apply an oscillating voltage between the electrodes



- the resulting potential is :

$$\varphi(x, y, z, t) = (U_{DC} + V_{AC} \cos\Omega t) \frac{x^2 + y^2 + 2z^2}{2r_0^2}$$





B. Operation of Paul trap



www.nobelprize.org



B. Motion of a single trapped ion

$$\varphi(x, y, z, t) = (V_{DC} + V_{AC} \cos\Omega t) \frac{x^2 + y^2 + 2z^2}{2r_0^2}$$

The motion of a single particle with e/m evolving in this potential is described by

$$\frac{d^2 u}{dt^2} + \frac{\Omega^2}{4} (a_u - 2q_u \cos \Omega t) u = 0 \qquad \text{for } u=x,y,z$$

with
$$a_X = -\frac{a_Z}{2} = \frac{8eU_{DC}}{2r_0^2m\Omega^2}$$
 and $q_X = -\frac{q_Z}{2} = \frac{4eV_{AC}}{2r_0^2m\Omega^2}$

→ Mathieu equations



MÉMOIRE

SUR

LE MOUVEMENT VIBRATOIRE

D'UNE MEMBRANE DE FORME ELLIPTIQUE;

PAR M. ÉMILE MATHIEU [*].

Imaginons une membrane tendue également dans tous les sens, et dont le contour, fixé invariablement, est une ellipse. Notre but, dans ce Mémoire, est de déterminer par l'analyse toutes les circonstances de son mouvement vibratoire; nous y calculons la forme et la position des lignes nodales et le son correspondant. Mais ces mouvements sont assujettis à certaines lois générales qui peuvent être définies sans le secours de l'analyse.

Lorsqu'on met la membrane elliptique en vibration, il se produit deux systèmes de lignes nodales qui sont, les unes des ellipses, les autres des hyperboles, et toutes ces courbes du second ordre ont les mêmes foyers que l'ellipse du contour.

Tous ces mouvements vibratoires peuvent être partagés en deux genres. Dans l'un de ces genres, le grand axe reste fixe et forme une ligne nodale, et si l'on considère deux points symétriques par rapport au grand axe, leurs mouvements sont égaux et de sens contraire. Dans l'autre genre, au contraire, les extrémités du grand axe situées entre les foyers et les sommets forment des ventres de vibration, tandis que la partie située entre les deux foyers offre un minimum de vibration,

[*] Ce Mémoire a été exposé au mois de janvier 1868 dans un cours à la Sorbonne.

Tome XIII (2e série). - Avail 1868.

E Mathieu, J Appl Math, 1868

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The motion of a single particle with e/r



with
$$a_X = -\frac{a_Z}{2} =$$

→ Mathieu equat

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B. Mathieu equations

The motion of a single ion e/m evolving in this potential is described by

for u=x,y,z
$$\frac{d^2u}{dt^2} + \frac{\Omega^2}{4} \left(a_u - 2q_u \cos \Omega t\right)u = 0$$

with
$$a_x = -\frac{a_z}{2} = \frac{8eU_{DC}}{2r_0^2m\Omega^2} \qquad q_x = -\frac{q_z}{2} = \frac{4eV_{AC}}{2r_0^2m\Omega^2}$$

stability of the solution only depends on e/m, r_0, $\Omega,$ U_{\rm DC} and V_{\rm AC}

stability diagram



B. Stability diagram of Mathieu equations

$$a_{x} = -\frac{a_{z}}{2} = \frac{8eU_{DC}}{2r_{0}^{2}m\Omega^{2}} \qquad q_{x} = -\frac{q_{z}}{2} = \frac{4eV_{AC}}{2r_{0}^{2}m\Omega^{2}}$$





B. Stability diagram of Mathieu equations





B. Stability diagram of Mathieu equations

$$a_{x} = -\frac{a_{z}}{2} = \frac{8eU_{DC}}{2r_{0}^{2}m\Omega^{2}} \qquad q_{x} = -\frac{q_{z}}{2} = \frac{4eV_{AC}}{2r_{0}^{2}m\Omega^{2}}$$





B. Frequencies of motion

exact solutions of the Mathieu equations are

$$u(t) = A \sum_{n=-\infty}^{\infty} C_{2n} \cos(\beta + 2n) \Omega t/2 + B \sum_{n=-\infty}^{\infty} C_{2n} \sin(\beta + 2n) \Omega t/2$$

- where A and B are constants depending on initial conditions. The coefficients C_{2n} , which are the amplitudes of the Fourier components of the particle motion, decrease with increasing n.

 $\omega_u =$

 β can be exactly determined by

$$\beta_{u}^{2} = a_{u} + \frac{q_{u}^{2}}{(\beta_{u} + 2)^{2} - a_{u} - \frac{q_{u}^{2}}{(\beta_{u} + 4)^{4} - a_{u} - \frac{q_{u}^{2}}{(\beta_{u} + 6)^{2} - a_{u} - \dots}} + \frac{q_{u}^{2}}{(\beta_{u} - 2)^{2} - a_{u} - \frac{q_{u}^{2}}{(\beta_{u} - 4)^{2} - a_{u} - \frac{q_{u}^{2}}{(\beta_{u} - 6)^{2} - a_{u} - \dots}}$$



B. Motion of the single particle

for the large majority of cases the adiabatic approximation is sufficient:

for $q_u < 0.4$ and $a_u \ll q_u$

h
$$u(t) = R_u \cos \omega_u t \left(1 + \frac{q_u}{2} \cos \Omega t\right)$$

h $\omega_u = \frac{1}{2} \beta_u \Omega$ and $\beta_u = \sqrt{a_u + \frac{q_u^2}{2}}$

with

H.G.Dehmelt, *Radiofrequency spectroscopy of stored ions I: storage* Advances in Atomic and Molecular Physics **3**, 53-72 (1967)



B. Motional frequencies

$$u(t) = R_u \cos \omega_u t \left(1 + \frac{q_u}{2} \cos \Omega t\right)$$

qz = 0.22

- harmonic oscillation
- secular motion $\omega_{\!_{\rm u}}$ and micro-motion Ω





B. Motion of the single particle

for $q_u < 0.4$ and $a_u < < q_u$

$$u(t) = R_u \cos \omega_u t \left(1 + \frac{q_u}{2} \cos \Omega t\right)$$

with

$$u_u = rac{1}{2} eta_u \Omega$$

and

$$\beta_{u} = \sqrt{a_{u} + \frac{q_{u}^{2}}{2}}$$

!! Values diverge rapidly for q > 0.4 **!!**

A better approximation can be found in

J.P.CARRICO Applications of inhomogeneous oscillatory electric fields in ion physics Dyn.Mass Spectrom. **3**, 1-65 (1972)

$$\beta_{\xi} \approx \left[a_{\xi} - \frac{(a_{\xi}-1) \cdot q_{\xi}^{2}}{2(a_{\xi}-1)^{2} - q_{\xi}^{2}} - \frac{(5a_{\xi}+7) \cdot q_{\xi}^{4}}{32(a_{\xi}-1)^{3}(a_{\xi}-4)} - \frac{(9a_{\xi}^{2}+58a_{\xi}+29) \cdot q_{\xi}^{6}}{64(a_{\xi}-1)^{5}(a_{\xi}-4)(a_{\xi}-9)}\right]^{1/2}$$



C. Strong confinement

$$u(t) = R_u \cos \omega_u t \left(1 + \frac{q_u}{2} \cos \Omega t\right)$$

- the amplitude of the ion motion increases with the distance from the trap center
- only in the trap center r=0 can it be 0
- harmonic oscillator in a potential well of limited length
- \rightarrow discretisation of frequencies (energy levels)
- ◆ if amplitude of motion R_u is smaller than $\lambda/2\pi$ → discrete spectrum for $\omega_u > \gamma$
- for a given energy (Doppler limit) : R_u is smaller for higher motional freq.s $\omega_u/2\pi \gg 1 \text{ MHz} \rightarrow \Omega/2\pi \gg 10 \text{MHz}$

→ single ion(s) in miniature traps





C. Lamb-Dicke regime

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DW Wineland & W Itano, Phys. Rev. A **20**, 1521-1540 (1979), Phys. Today, pp. 1-8 (1987)

Single ions or electrons

Schroedinger 1952:

Erstens ist es angemessen festzustellen, dass wir mit einzelnen Teilchen nicht EXPERIMENTIEREN, ebensowenig wie wir Ichtyosaurier im Zoo züchten können. Wir prüfen Spuren von Ereignissen, lange nachdem sie stattgefunden haben...

First it has to be stated, that we do not EXPERIMENT with single particles, as much as we do not raise ichtyosauri in a zoo. We look for evidences of facts, long after they have happened

Zweitens … ist… die Tatsache …zuzugeben, dass wir nie mit **EINEM** Elektron, Atom oder (kleinen) Molekül experimentieren. In Gedankenexperimenten geben wir manchmal vor, es zu tun, allerdings stets mit lächerlichen Konsequenzen.

Second, the fact is, that we never experiment with a SINGLE electron, atom, or (small) molecule. In gedankenexperiments, we sometimes pretend to do so, but always with ridiculous consequences





Visual observation of a single Ba⁺ - ion



Abb. 1.2: Optischer Nachweis eines einzelnen Bariumions in einer Paul-Falle.

Experiment Heidelberg, Toschek group, 1980

Neuhauser et al., Localized visible Ba⁺ mono-ion oscillator, Phys Rev A 22, 1137 (1980)





D. More than ion

space charge effects

- limit the ion density to 10⁶/cm³
- shift the frequencies of motion to lower values (depending on the geometry of trap and size of cloud)
- distort the observed stability diagram



D. Spatial and density distribution of an ion cloud



Fig. 1.7. (a) Fluorescence $I_{\rm F}$ of Ba⁺ ions in axial and radial direction in a Paul trap of 4 cm ring radius showing a Gaussian density distribution [10]. (b) Calculated density distributions for different ion temperatures [11]

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Chrs

H. Schaaf, U. Schmeling, G. Werth,
 L.S. Cutler et al.,

 Appl. Phys. 25, 249 (1981)
 Appl. Phys. B 36, 137 (1985)



D. Density distribution of an ion cloud





D. Optimal trapping point

Ifflaender and Werth, Metrologia 1977



Fig. 3. Computed iso-density lines. Dotted lines: boundary of stable region

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E. Characterisation of ion trap

R Alheit et al., Appl. Phys.B. 61, 277-283 (1995)

- number of stored ions
- maximum 5000 ions







E. Instabilities in an ion trap

R Alheit et al., Appl. Phys.B. 61, 277-283 (1995)

- number of stored H2+ ions





E. Instabilities in an ion trap

work by Dawson&Whetten, IJMSIP (1969), Vedel et al., IJMSIP (1990), Morand et al, Mass Spectrom. 1991 and Guidugli&Traldi, Mass Spectrom.

Wang, Franzen &Wanczek, IJMS (1993) showed that for a 3D trap in the first stable region ($\beta_r > 0$, $\beta_z < 1$)



also coupling between macro- and micromotion produces « black holes » for higher-order contributions

for example $\beta_z = 1/2$ (octupole) or $\beta_z = 2/3$ (hexapole)

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E. Instabilities in an ion trap

R Alheit et al., Appl. Phys.B. 61, 277-283 (1995)

for example N=4

 β_r =1/2 ; β_z =1/2

1/2 β_z +3/2 β_r =1

 $3/2 \beta_z + 1/2 \beta_r = 1$

 $\beta_z + \beta_r = 1$

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Nonlinear resonances – used for isotope separation

R. Alheit, K. Enders, G. Werth, Appl. Phys.B 62, 511-513 (1996)



Ejection with tickle



F Vedel, M Vedel, RE March, IJMSIP 99, 125 (1990)



Ejection with tickle




Detection of image currents



Image from K Blaum



Detection of image currents



circuit G Werth





Cloud with "tickle"

- Additional small amplitude exciting secular frequencies
- → heating



Tickle frequency $\boldsymbol{\omega}$

NON - DESTRUCTIVE



Characterization of the miniature trap

application of an additional V_{AC}-voltage of small amplitude (« tickle »)



• for the Paul-Straubel case: $a_z = \frac{8eU_{DC}}{mr_1^2 \Omega^2 \mathcal{L}}$ and $q_z = -\frac{4eV_{AC}}{mr_1^2 \Omega^2 \mathcal{L}}$

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- different geometric defects lead to : $a_z \mathcal{L}_z = -2a_x \mathcal{L}_x$ and $q_z \mathcal{L}_z = -2q_x \mathcal{L}_x$
- for $580V_{rms} \le V_{AC} \le 790V_{rms}$: $8.0 \ge L_z \ge 7.6$ and $7.0 \le L_x \le 7.1$

Martina Knoop – Jan 2018

Stability diagram: limits and canyons

• scan of the applied continuous voltage U_{DC} gives information about the confinement efficiency of the trap without any external perturbation

•« black canyons » can be followed through the stability diagram







2nd part of lecture



F. Modified geometries







Linear ion trap – Paul's mass filter !

- extend along the *z*-axis
- add end electrodes



 \rightarrow a line where the potential is 0 !



picture K Blaum⁴⁴

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RF field yields transverse pseudopotential



slide M Drewsen

The Aarhus linear Paul trap



Sinusoidal RF potential: $U_{RF}(t)=U_{RF}sin(\Omega t)$

Effective oscillation freq.'s: $\omega_r = 1/2 \ \beta \ \Omega, \quad \beta = (1/2 \ q^2 + \Omega)^{1/2}$ $\omega_r = (-1/2 \ \alpha)^{1/2} \Omega$ Stability parameters:

$$\mathbf{q} = \frac{4\mathbf{Q}\mathbf{U}_{\mathsf{RF}}}{\mathbf{m}\Omega^2 \mathbf{r}_0^2} \quad \mathbf{a} = -\frac{\alpha \mathbf{Q}\mathbf{U}_{\mathsf{end}}}{\mathbf{m}\Omega^2 \mathbf{r}_0^2}$$

Atomic density:
$$n_i = (\epsilon_0 U_{\rm rf}^2)/(M_i r_0^4 \Omega^2)$$

slide M Drewsen



• symmetric stability diagramm





Harmonic linear Paul trap: Stability diagram and effective potentials, M. Drewsen and A Broner, Phys Rev A 62, 045401 (2000) !! some errors!!

• shape of the rods



Reuben et al., *Ion trajectories in exactly determined quadrupole fields*, IJMS 154, 43-59 (1996)







Crystals

••		
	• •	
• •		Oxford
••		
••		
••		

Innsbruck









The race-track trap

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un

slide courtesy M Drewsen

Observation of multi-shell structures in a quadrupole storage ring



2

The ion circus

CSNSM

The ion circus project

- The ion circus is a circular Paul trap that can simultaneously cool and mass separate isobaric nuclides.
- The resolving power is increased as the ions orbit in the ring. Since they are buffer-gas cooled, the transmission is not degraded



The ion circus

CSNSM



Main characteristics

Goal m/ Δ m=5000

- The ion circus is composed of 36 segments of radiofrequency quadrupole mass filter bent into a circle
- Ring diameter : 400 mm
- Distance between two opposite electrodes : 10 mm
- Acceptance : 3 mm
- Energy @ injection : 100 <> 1500 eV
- Frequency ≃ 2 MHz
- Potential on electrodes : +/- 500 V
- Time of trapping <1 s
- Energy @ ejection : a few eV

« *The ion circus: A novel circular Paul trap to resolve isobaric contamination* » E. Minaya Ramirez, S Cabaret, D Lunney, NIM B 266, 4460-4465 (2008)

The ion circus



Main challenge:

capacity of electrodes

ions injected from an external source.





2k-pole traps





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2k-pole traps

Pseudo-potential $V^*(r) = rac{k^2 q^2 V_0^2}{16m\Omega^2 r_0^2} \left(rac{r}{r_0}
ight)^{2k-2}$





 $rac{q\kappa V_{end}}{2z_0^2} (2z^2-r^2)$

• stability of the trajectories governed by Mathieu's equations

• Mathieu parameter

- non-linear dynamics.
- no more exact stability criteria and sensibility to initial conditions
- adiabaticity parameter $\eta_{ad}\left(r
 ight)$ empirically limited to $\simeq 0.36$



Motion in a multipole

- In the radial potential
- Molecular Dynamics to accompany the evolution of structures
- Monte-Carlo methods for crystal structures





Non-neutral plasma (cold charged fluid)



Non-neutral plasma (cold charged fluid)



Radial potential $V^*(r) \propto r^{2k-2}$

Potential well depth $V^*(R_{max}) \propto k^{-2}$



22 pole trap D Gerlich, Uni Chemnitz, Germany

Adv Chem Phys <u>LXXXII</u>, 1 (1992)







2k-poles

- Less rf heating
- Creation of different (crystal) structures : tubes, rings
- Symmetric structures (2D)

8888

- ?? Trapping range, initial conditions
- Laser power
- Detection efficiency









Miniature traps



Systematic effects - experimental constraints -

 $\Delta v_{nat} / \nu \approx 3 \cdot 10^{-16}$

to resolve 1Hz at 411 THz $(2.4 \cdot 10^{-15})$:

ion cooled to Doppler limit, <n>≈10</n>	Doppler 2 nd order	
a magnetic field < (0.1 \pm 0.05 μ T)	quadratic Zeeman quadratique, AC Stark	
a residual electric field <1V/mm	DC Stark	
gradient of electric field <1V/mm over 1 mm (spherical traps)	quadrupole moment	
3 optical axis (orthogonal)	measurement of quadrupole moment	
T= 300K	BBR	
P<0.75μW/mm² @ 729nm	AC Stark (light shift)	





Miniature traps

to reach strong confinement at Doppler limit

- \rightarrow need high motional frequencies
- → requires high trapping frequencies ($\Omega/2\pi$ > 10 MHz) with nonnegligeable amplitudes (a few 100 V)

$$q_{x} = -\frac{q_{z}}{2} = \frac{4eV_{AC}}{2r_{0}^{2}m\Omega^{2}}$$
reduce r

« Novel miniature ion traps », Schrama et al., Opt. Comm 101, 32-36 (1993) - shows that if the potential is harmonic in the central 10% of the structure this is largely sufficient for a single ion !

Martina Knoop – Jan 2018



The stylus trap (or 4 π trap)







a

h



Figure 3 | **Potential applications of the trap geometry. a**, Placement of the ion in the focus *f* of a parabolic mirror with depth *z* to maximize photon-ion coupling. **b**, Scanning of different surfaces with the ion as a sensitive probe.





Stylus ion trap for enhanced access and sensing ^{1.0} ^{0.5} Robert Maiwald, Dietrich Leibfried, Joe Britton, James C. Bergquist, Gerd Leuchs and David J.Wineland, Nature Physics 2009, DOI: 10.1038/NPHYS1311

Microfabricated traps

• scalable architectures

D.Kielpinski, C. Monroe, and D. J.Wineland, Nature 417, 709 (2002)

"quantum CCD" architecture - Wineland et al. (1998)



and
$$\omega_r = \frac{eV_{AC}}{\sqrt{2} m\Omega d^2}$$

with d the distance to the electrodes





Microfabricated traps







slide U Tanaka

Microfabricated surface traps

Simulated pseudopotential



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Microfabricated surface traps



Microfabricated surface traps

Simulated pseudopotential - dc dependence -


Micro-traps with junctions multiplexer 4k 0.1: Mary Rowe et a 1.5 cm 200 µm W. K. Hensinger 49-electrode S. Olmschenk 11-zone D. Stick T-junction D. Hucul M. Yeo typical ion J. Rabchuck C. Monroe spacing $\cong 2 \,\mu m$ mm 00 m 400µm Aix*Marseille 73 CNTS 73

NIST trap



slide Didi Leibfried

NIST race-track



Mainz trap

Mainzer segmentierte Mikrofalle





S. Schulz, F. Schmidt-Kaler Physik in unserer Zeit, Vol. 38, 162 (2007)

slide Ferdi Schmidt_Kaler

Mainz trap

segmentierte Mikrofalle

- Ti/Au on Al₂O₃-Wafer (10nm/400nm)
- fs-Laser Schnitt in Au/Ti and Al₂O₃
- Justage und
- Fixierung in den Chiphalter
- bonding





Elektronen-Mikroskop Aufnahme

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Motional heating

Heating rate orders of magnitude over Johnson noise, physical origin unknown



Combining ion trap and cavity

G. R. Guthöhrlein, M. Keller, K. Hayasaka, W. Lange, H. Walther, Nature 414, 49 (2001)



Integrated fibers



W. Lange, Univ Sussex

Fluorescence detectionCavity





