lecture 20.10.2011 we had in the last week:

- introduction into atomic physics, relevance
- introduction into cluster physics

today:

- few more remarks on cluster physics
- atomic physics: history
- Doppler-free spectroscopy
- preparation of atomic beams

A cluster of simple metal atoms can be considered as a metallic quantum dot. In the corresponding bulk materials the electrons need much more space.



size-dependence

Full-shell Clusters	Total Number of Atoms	Surface Atoms (%)
1 Shell	13	92
2 Shells	55	76
3 Shells	147	63
4 Shells	309	52
5 Shells	561	45
7 Shells	1415	35

Electronic shell structure of metal clusters

58 (2)----330 Al110 example: Al_N 3 electrons per atom **3g** (18) **318** Al106 2i (26) _____300 Al100 1k (34) 274 Al91-4p (6) -----240 Also 3f (14) _____234 Al78 Al73-Al66 4s (2)------168 AI56 Al55* **Al**52 1i (26) 138 Al46 Al37-2f (14) _____106 Al35* will be derived later 1h (22) _____92 38 (2) 70 Al23⁻ in this lecture 2d (10) _____68 1g (18) -----58 Al₁₉. **2D** (6) **_____40** Al₁₃-1f (14) ______34 Al11-**2s** (2) **_____20** 1d (10) ______18 1p (6) ------8 **1s** (2) _____ 2

FIG. 1. Spherical shell closings and the corresponding closed shell neutral and negative clusters of trivalent A1. The number in the parentheses after each shell index indicates the occupation number, 2(2l + 1).

electronic levels revealed by photoelectron spectroscopy





Hakkinenet al., PRL 93 093401(2004)

FIG. 1. Photoelectron spectra of Cu_n^- , Ag_n^- , and Au_n^- (n = 53, 55, 57, 58) obtained at a photon energy of 6.42 eV.

Physical nature of clusters may change with size

Example: Electronic states in Magnesium from the atom to bulk. Metallic behaviour stets in when the full s-band starts to overlap with the empty p-band



atomic physics - the beginning

- Leuklipp 440 v Chr, Demokrit 460-370 v Chr ατομοσ 'completely undivisible' (gänzlich unteilbar). idea: outside the atom emty space
- Epikur 341-271 v Chr: atom -- gravity (Schwere)
- later the idea of 'atom' has been forgotten for centuries
- for the church the reinvention of the atom has been too materialistic; in 1348 Nicolas von Antrecourt had to retract (widerrufen) his ideas on the atomic nature
- break-through from the 17th century on mainly by chemists (weighing, reactants and products)
- 19. Jht. Clausius, Maxwell, Boltzmann: p, T, specific result from atomic cillisions

historical key experiments still important today

another Millikan experiment: magnetic levitation spectrometer



measure the oscillation period and amplitudededuce the charge state with extremely high precision

Morpurgo et al., Nucl. Inst. Meth. 79 (1970) 95

modern Millikan experiment with magnetic levitation

Electric Neutrality of Matter

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Sezione di Genova, Italy

(Received 18 April 1977)

With the use of a new feedback levitation electrometer (with an increase in sensitivity by 10^3 in comparison to our previous graphite experiments) iron objects of mass $\sim 2 \times 10^{-4}$ g have been explored for fractionally charged quarks and/or a possible electron-proton charge difference. Upper limits found were $N(\text{quarks})/N(\text{nucleons}) < 3 \times 10^{-21}$ and $(\mathcal{G}_{p} - |\mathcal{Q}_{e}|)/\mathcal{Q}_{p} < 10^{-21}$. The present "sensitivity" is $\sim 10^{7}$ times that of the original Millikan experiment. VOLUME 38, NUMBER 22 PHYSICAL REVIEW LETTERS

30 May 1977



- a) changes in the charge of a steel sphere with 3.3x10⁻⁵ g Residual charge smaller than 1/40 e
- b) rotating cylinder with 2.5 x 10⁻⁴ g.
 Charge changes from +1 to -1 and -2

conclusions:

- upper limit N(quarks)/N(Nucleons) smaller than 3x10⁻²¹
- $(Q_p-Q_e)/Q_p$ smaller than 10^{-21}
- sensitivity 10⁷ times Millikan

Basics of atom (and molecular) spectroscopy how to overcome effects of motion and collisions

one aim: to do undisturbed spectroscopy to learn, e.g., about line widths (lecture by Prof. Bauer)

- Doppler-reduced spectroscopy
- supersonic atom beams

In the laboratory frame: angular frequency $\boldsymbol{\omega}$.

In a reference frame of an atom moving with a speed **v**: angular frequencies ω' or ω'' .

<u>solution 1</u>: Doppler-free spectroscopy for example *Two-photon spectroscopy*



If the atom absorbs one photon from each of the counter-propagating beams then the Doppler shifts cancels in the rest frame of the atom

$$\omega(1+\frac{v}{c}) + \omega(1-\frac{v}{c}) = \omega$$

there are many more methods of Doppler-free spectroscopy

1

<u>solution 2</u>: cold atom beams for example *crossed beams technique*





thus: we have to create ultracold atomic beams

The **analysis of compressible fluid flow** involves four equations of particular interest: Energy - Continuity - Momentum - The equation of state

Conservation of energy, isentropic flow (no heat exchange, no friction) between x1 and x2:



1]

$$h_{1} - h_{2} = \frac{1}{2} \left(\sqrt{2^{2} - \sqrt{1^{2}}} \right) = C_{P} \left(T_{1} - T_{2} \right)$$
 [eq.

Enthalpy h, v velocity in x-direction, Cp heat capacity, T1, T2 temperatures at x1, x2.

Change (decrease) in enthalpy is equal to the change (increase) in kinetic energy
 ▶ heat of the fluid is being used to accelerate the flow!

For isentropic flow: temperature, pressure, and fluid density $\boldsymbol{\rho}$

$$\frac{T_{\circ}}{T} = \left(\frac{P_{\circ}}{P}\right)^{\frac{k-1}{k}} = \left(\frac{\rho_{\circ}}{\rho}\right)^{k-1} \text{ [eq. 2], with k: ratio of specific heats } k \equiv \frac{C_{P}}{C_{v}} = \frac{C_{P}}{C_{P}-R}$$

and R = R'/mol.weight, R': Avogadro's constant

application to nozzle flow



role of the Mach number

a: local sonic velocity

M: the Mach number (ratio of the flow velocity to the local sonic velocity)

$$a = \sqrt{kRT}$$
 $M = \frac{v}{a}$ [eq. 3]

From eq. 1, 2, and 3 we derive

$$\frac{T_{\circ}}{T} = 1 + \frac{k-1}{2} M^2$$
 [eq. 4]

Further considerations: From [eq. 4], the first law $\frac{P}{\rho^{k}}$ = constant, and the eq. of state $P = \rho R T$:

$$\frac{\mathsf{P}_{\circ}}{\mathsf{P}} = \left(1 + \frac{\mathsf{k} - 1}{2} \mathsf{M}^2\right)^{\frac{\mathsf{k}}{\mathsf{k} - 1}}$$

$$\frac{\omega_0}{\omega} = \left(1 + \frac{k-1}{2} M^2\right)^{\frac{1}{k-1}}$$

In our case: T_0 , P_0 , ρ_0 the values before expansion

consequences for the atomic beam



original work: Andersen and Fenn, The physics of fluids 8 (1965) 780

preparation of ultracold atomic beams by supersonic jet expansion



Fig. 8: Die mikroskopische Ursache für die Temperaturerniedrigung und Clusterbildung bei der adiabatischen Expansion [13]. Im Ausgangsbehälter herrscht vor der Expansion thermisches Gleichgewicht. Die ungerichtete Geschwindigkeitsverteilung der Teilchen ist durch die Maxwellverteilung bestimmt. Bei der Expansion des Gases durch eine Düse kommt es durch Stöße mit den anderen Gaspartikeln zur Abnahme der inneren Energie zu Gunsten der Expansionsgeschwindigkeit u. Die Relativgeschwindigkeit im kalten Molekularstrahl nimmt stark ab, wodurch die "kalten" Atome zu Clustern zusammenlagern.

technical realization of an atomic beam



Expansion (Huge pressure drop $>10^3$)

supersonic jet expansion



acceleration in nozzles (simulated)



- 1. expansion shown for Argon
- the gas reaches 600m/s over a distance of 2 nozzle diameters in 1 μs
- 3. the acceleration is enormous:

a>5*10⁸ m/s² for Argon a>5*10⁹ m/s² for Helium

Interesting inertial effects in spectroscopy??