Introduction to Physics of Nanosystems

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2007 Nobel Prize in physics:



Albert Fert Peter Grunberg (France) (Germany)

... for discovery of the phenomenon of "giant magnetoresistance", in which weak magnetic changes lead to big differences in electrical resistance.

First Nobel Prize in physics for nanotechnology!

GMR: discovered in 1988

The discovery has allowed industry to develop sensitive reading tools to pull data off hard drives in computers and other digital devices.

Radical miniaturization of hard disks

last years.



Onset of SPINTRONICS!

Applications:

- IBM 1997: reading data off CD,
- angle, position, velocity spin sensors (ABS: Antiblock Braking System)
- Motorola: MRAM (Magnetoresistance Random access Memory)
- HDTV, DVD recorders, ...

Microsystems:

- atomic nuclei
- atomic clusters
- carbon nanosystems
- quantum dots
- heterostructures
- Bose-Einstein condensate
- optical lattice

Related fields and phenomena:

- quantum transport,
- spintronics,
- Hall effect

$$\begin{cases} 10^{-15} m \\ 10^{-9} m & - nano \end{cases} \begin{array}{c} 10^{-9} = micro \\ 10^{-9} = nano \\ 10^{-12} = pico \\ 10^{-15} = femto \\ 10^{-18} = atto \end{cases}$$

$$10^{-3} - 10^{-6} m$$

- new generation of lasers (ft, at)
- laser cooling

New systems phenomena techniques were produced 5 - 20 years ago

Variety of actual micro- and nano-systems



For every nanosystem:

- definition
- how to produce
- main properties and physical effects
- why it is interesting for:
 - fundamental physics
 - applications

Lecture 1: Atomic clusters

- metal clusters
- similarity with nuclei
- quantum shells and supershells
- dipole plasmon
- applications

Lecture 2:

Theoretical models

- Kohn-Sham functional Carbon nanosystems
 - fullerenes
 - graphene
 - nanotubes

Lecture 3: Quantum dots

- Wigner molecules
- Coulomb blocade
- spintronics

Heterostructures

- Giant Magnetoresistance (Nobel -2007)

Quantum transport

- different kinds of QT Biomedical applications
 - cancer diagnostic and therapy

Lecture 4:

Bose-Einstein condensate

- amazing laboratory for new physics Optical lattice Nano in Russia and Dubna Conclusions

ATOMIC CLUSTERS

- variety of atomic clusters,
- cluster production,
- metal clusters: mean field,
- similarity of atomic clusters and nuclei
- quantum shells, magic numbers,
- super-shells,
- deformation,

- temperature effects,
- phase transitions,
- dipole plasmon, experiment,
- spill-out,
- applications,
- theoretical methods: Kohn-Sham functional, ...

Atomic clusters

- * Atomic cluster is a bound system of identical atoms.
- * Bridge between one atom and bulk:

* Now it is possible to produce clusters with any number of atoms and for any element of the periodic table. Fundamental physics + applications!

- * The most interesting size interval is 1<N<1000.
- * Applications:
- -- creation of new materials by cluster deposition,
- -- catalysis of chemical reactions,
- -- new alloys,
- -- new magnetic materials,
- -- cluster nano-electronics,
- -- clusters to cure cancer.







Cluster production 1. W.D. Knight, et al, PRL <u>52</u>, 2141 (1984) -- experiment 2. W. Ekardt, PRB, 1558 (1984) -- theory

Seeded supersonic nozzle source



- heating of the material in reservoir to get the supersaturated vapor,
- mixture with a beam of high-pressure inert gas,
- supersonic expansion of the mixture to vacuum,
- sudden expansion, cooling and condensation of atoms into clusters,
- ionization of neutral clusters in beam by laser,
- detection and separation of clusters with a given number of atoms,
- experiments in a beam of size-separated clusters.

Alternative sources: creation of supersaturated vapor by intense laser, growing cluster in solutions, ...

Alternative methods of cluster production



Clusters in our life

Colloidal gold: known in ancient Egypt

Gold clusters:

- stained-glass windows in cathedrals:

Metallic micro-grains added to the glass result in various colors of the penetrated light. The light wave length depends on the kind of the metal and grain size.

- British museum, Licurgus cup, IV century AD

The green cup becomes red if to light it from inside (the glass with colloidal gold and silver)

Silver clusters: photography:

Silver films used in photography consist on silver clusters.

Different kinds of powders.

Clusters as small metal particles are known since ancient times but only ~ 25 years ago we have mastered production of small clusters with given number of atoms.



Metal clusters: mean field, quantum shells, magic numbers



The remaining difference in magic numbers is caused by a weak spin-orbital splitting in electronic systems.

Metal clusters

- 1. W.D. Knight, et al, PRL <u>52</u>, 2141 (1984) -- experiment
- 2. W. Ekardt, PRB, 1558 (1984)

-- theory

* Clusters of some metals (alkali and noble) are very similar to atomic nuclei.

* Two subsystems in metal clusters:
 -- valence electrons (quantum properties),

-- ions (classical particles).

* Mean free path of valence electrons is of the same order of magnitude as the cluster size. So their motion can be quantized and they can create the mean field of the same kind as nucleons do in atomic nuclei.

in metal clusters





Metal clusters vs nuclei

Similarities:

- Mean field, quantum shells, magic numbers
- Various deformations: L=2,3,4,...
- Shape isomerism
- Collective modes:
 - plasmons +---> giant resonances
- Fission and fusion
- ...

and differences

- More quantum shells, supershells
- Neutral, negative/positive charges
- Free, supported, embedded, ...

Metal clusters

"Quantum" valence electrons and "classical" ions

$$E = \frac{p^2}{2m} = \frac{\hbar^2}{2m} (\frac{\partial}{\partial x})^2 \approx \frac{\hbar^2}{2m} (\frac{1}{\Delta x})^2$$

 Na_{20} : $\Delta x \approx D \approx 11\dot{A}$

1K=8.6 · 10⁻⁵eV

temperature:	$t \approx 100 - 800 \text{ K} \approx 0.01 - 0.1 \text{ eV}$			
electrons:	$E_e \approx 0.06 eV \ge t$ quantum particles			
ions:	$E_i \approx 0.06 \cdot 10^{-3} \text{ eV} < t \iff \text{ classical particles}$			

So, just valence electrons determine quantum properties of clusters while ions can be treated as classical particles.

In metal clusters like Na ones, the ions can be safely replaced by the uniform frozen distribution of the positive charge:

jellium approximation

Metal clusters: deformation

$$R = R_0(\delta_0 + \frac{\delta_{20}}{\gamma_{20}}(\Omega))$$

2.0 2.5 3.0 3.5

AW [eV]

Like atomic nuclei, metal clusters with closed (fully occupied) quantum shells are spherical while clusters with open (partly occupied) quantum shells are deformed.



Coexistence of different cluster shapes.

Limits for the number of quantum shells (1)

How many quantum shells can exist in metal clusters?

Is there any upper limit?

If yes, then what is a physical reason for the limit?

Limits for the number of quantum shells (2)



Limits for the number of quantum shells (3)

Shell number (N)	Theory (Nishioka)	Exper. (Pedersen)	Exper. (Schmidt)	
1	2	2	2	
2	8	8	8	
3	20	20	18/20	
4	40	40	34/40	
5	58/68	58	58	
6	92	92	90/92	
7	138	138	138	
8	198	196	198±2	
9	254/268	264	263±5	
10	338	344	341±5	Quantum shells
11	440	442	443 ± 5	(best for high T)
12	562	554	557±5	(best for high f)
13	694	680	700 ± 15	
14	832	800	840 ± 15	
15	1012	970	1040 + 20	
16	1100	1120		
17	1216		1220 ± 20	
18	1314	1310	1430±20	
19	1.516	1500	1980*	$\overline{}$
20	1760	1780	2820*	
21	2048	2040	3800*	
22	2334/2368	2370	5070*	Coometrical
23	2672	2720	6550*	Geometrical
24	3028		8170*	> (icosahedron)
25	3438	-	10200*	
26	3848		12500*	5110115
27	4154		15100*	like in the bulk!
28			18000*	(bact for low T)
29			21300*	
		T = 800 K	T = 100 K	

magic numbers

Supershells (1)

Theory of periodic orbits

R. Balian and C. Bloch, Ann. Phys., 69 (1971) 430.



Quantum shell

Periodic orbit

 $(\Delta I, \Delta n) \Longleftrightarrow (k, m)$

k – number of contacts m – number of revolutions

Quantum shells in finite systems have a classical analog in the form of periodic closed orbits in the spherical vibrator.

Temperature destroys the orbits so as only a couple of simple orbits with similar characteristics survives: (3,1), (4,1).

$$\cos(\omega_{31}t) + \cos(\omega_{41}t)$$

$$= 2\cos(\frac{(\omega_{31} - \omega_{41})t}{2})\cos(\frac{(\omega_{31} + \omega_{41})t}{2})$$

low frequency high frequency

Beating! Supershells !!!



Density of levels in sodium cluster with 3000 atoms.



Supershells (3)

Discovery of supershells in experiment for Na clusters:

J. Pedersen, S. Bjornholm, et al, Nature, <u>353</u> (1991).



This discovery leaded to a great progress of TPO, chaos/order studies, etc.

What we have learned from lecture 1:

- definition and variety of atomic clusters
- cluster production
- deformation / Jan-Teller effect
- mean field with quantum shells
- supershells

Similarity with nuclei only for a clusters of alkali and noble metals! For overwhelming majority of other clusters this similarity is absent. Thank you for your attention!