School on Shells Effects in Finite Quantum Systems (July 25-31, 2010)

Summary

The week-long School on Shells Effects in Finite Quantum Systems (50^{th} Course of the International School of Solid State Physics) took place at the renowned Ettore Majorana Centre for Scientific Culture in Erice, Sicily. It was attended by thirteen invited lecturers (theorists and experimentalists) and thirty-eight listeners, ninety percent of whom were graduate students and postdocs. The geographical diversity was quite remarkable: twenty-four countries were represented at the School. The directors/organizers of the Course were Vitaly Kresin (University of Southern California, Los Angeles, USA) and Klavs Hansen (University of Gothenburg, Sweden).

The School marked the twenty-fifth anniversary of the seminal discovery of a new manifestation of shell structure in nature: the observation of electronic shells in metal nanoclusters by the group of Walter D. Knight at Berkeley (it also commemorated this remarkable scientist on the tenth anniversary of his passing). The School's aim was to highlight the unity of physical principles that are now recognized to manifest themselves in a variety of systems (atoms, nuclei, clusters, confined quantum gases, nanostructures, quantum dots, and nanowires). These areas are very different in terms of energy scales and other physical characteristics, but their properties are strongly influenced by the quantization of motion of their constituent fermions. This was a central scheme of the School. Furthermore, as described in lectures, research has revealed productive connections with such fields as semiclassical quantization, level statistics and chaos, etc.

The diversity and the underlying universality of the physics presented at the School made it quite unique, and rewardingly interdisciplinary and synergistic. The listener evaluations were overwhelmingly positive, remarking on the overall high quality of the presentations and on the value of a broad introduction to the science of size-quantized systems. Furthermore, thanks to the allowance of time for personal discussions, there was abundant evidence of the School's serving to establish contacts, friendships, and – already - near-term collaborations.

Scientific Content and Discussion

The School set up a detailed web site, http://physics.usc.edu/Shells/. The site prominently acknowledges the sponsorship of the ESF/INTELBIOMAT program, as did the Book of Abstracts distributed to the participants.

The invited lecturers each presented two one-hour lectures (forty-five minute talks plus fifteen minutes allotted for discussions), divided over two consecutive days (see the schedule in the Programme section below). The subjects of the lectures were as follows (full abstracts are given in the Programme section):

(in alphabetical order)

Giorgio Benedek (University of Milano): *Shell effects in helium droplets*

Oriol Bohigas (University of Paris): *The compound nucleus, random matrix theories and chaotic dynamics*

Wolfgang Ernst (Graz University of Technology): *Shell models for alkali metal trimers: Electronic level structure and magnetic properties*

Laurent Gaudefroy (CEA/DAM Ile de France) and Alexandre Obertelli (CEA Saclay): *Developments in shell effect description of nuclear structure*

Claude Guet (CEA Saclay): *Linear and non-linear electron dynamics in finite systems*

Klavs Hansen (University of Gothenburg): *Thermodynamics of finite systems*

Walt de Heer (Georgia Tech): *Fundamentals of electronic shell structure in alkali clusters: Experiments and concepts*

Bernd von Issendorff (University of Freiburg): *Photoelectron spectroscopy of nanoclusters*

Vitaly Kresin (University of Southern California): *Long-range polarization interactions*

Mark Raizen (The University of Texas at Austin): *Comprehensive control of atomic motion*

Stephanie Reimann (Lund Institute of Technology): *Shells and spins in quantum dots, and from quantum dots to cold atoms*

Jan van Ruitenbeek (Leiden University): *Shell structure in metallic nanowires*

The schedule allowed for ample question time, and the lectures generated a large number of questions both n the lecture hall and during free discussion time, Most of the above presentations will be posted on the School web site as further reference for the listeners.

In addition, the listeners were encouraged to present posters describing their current work. Twenty-four posters were displayed during two poster sessions, and the comfortable environment of the Center and the allotment of discussion time enabled extensive and useful conversations among the participants at the poster sessions.

A questionnaire was handed out to the listeners on the last day. One of its sections asked for a set of grades. The results of the survey (31 responses) were as follows:

(1) How did you find the level of most lectures (0-5, 0=much too easy, 3=suitable, 5=far too difficult) - *Average grade 3.4*

(2) Was the format of the school appropriate with respect to the. length and distribution of lectures, time for questions and discussions, poster sessions, coffee breaks, etc. (0=all hopeless, 5=perfect) - *Average grade 4.7*

(3) Was the choice and relative weight of subjects useful for you (0=not all all, 5=perfect)? - *Average grade 3.5*

(4) Overall grade for the school (i.e., would you come again? 0=absolutely not, 5=absolutely yes) - *Average grade 4.3*

The organizers feel that this response, on the whole, validated their efforts to put together a survey Course aiming, so to speak, to help the attending graduate students and postdocs place their research into a broader scientific perspective; to expose them to the various experimental and theoretical techniques employed in the current research on finite Fermi systems in nanoscience, atomic, and nuclear physics; and (last but not least) to remind them of the beautiful unity of physics – a fact which is often mentioned in passing but is sometimes lost track of in the hustle, bustle, and drudgery of everyday research work.

The comments also suggested a number of logistical and other enhancements, which will of course be taken into account should the organizers decide to undertake the assembly of another School of this type.

It is worth noting that the Erice Centre hosted one of the first major international gatherings in the field of nanocluster science in 1987: 13th International Course on Solid State Physics, *Elemental and Molecular Clusters*. It was rewarding to use the occasion of the present 50th Course to review the progress achieved in the intervening years, and to highlight the various interconnections that have been established with other actively developing branches of physics.

In conclusion of this section, a comment from the aforementioned anonymous listener reviews: “The whole organization was very good! Thank you! And I highly appreciate the high 'social' degree of the event, it really was like a 'group' and not a collection of individuals." This was a gratifying remark, as a lot of planning and effort had been devoted towards trying to achieve this goal: to promote a community feeling among graduate students and postdocs engaged in research within this exciting field.

<u>Assessment</u>

As described in the preceding section, it is felt that the School largely succeeded in meeting its goals: to serve as an overview of the major concepts (both experimental and theoretical) underlying and unifying the study of size-quantized finite systems, and to stimulate a sense of community among the diverse international group of attendees. It also succeeded in promoting interaction and seeding actual collaborations. The listener reviews were positive and constructive. A number made personal comments along the lines of "… this has been one of the best summer schools I ever attended." The Summary section lists some of the participant statistics.

It should be emphasized that the quantum-scale phenomena addressed by the School have important practical implications within areas of relevance to the INTELBIOMAT program.

For example, there is currently a great deal of interest in the synthesis of novel materials utilizing nanoclusters as "superatom" building blocks based on the exceptional shell-based stabilities of particles of specific sizes. In fact, some researchers make the point that the ability to control the physics and chemistry of clusters by varying the number of their constituent atoms adds, in a way, a "third dimension" to the periodic table. Functional materials with tunable band gaps or collective (e.g., plasmonic) spectra are being discussed. Also, predictions have been made of the possibility of strong superconducting pairing in certain finite nanoclusters, deriving from the shell structure ordering of their electronic states.

Analogously, shell effects deriving from size quantization have attracted attention in studies of low-dimensional electronics systems, such as quantum dots and nanowires.

Nuclear physics is of great significance for several reasons. It is a stage where ground- and excited-state shell effects are famously important and have been addressed using a variety of ingenious many-body theoretical techniques. In addition to the fundamental importance of this field, it is of course of great relevance for its energy generation potential.

Cold quantum atomic gases is a "hot" field where shell effects, both of the constituent atoms and of the collective states, are of importance. It is noteworthy, in the context of the INTELBIOMAT program, that these atom-based systems have proven to be superb laboratories for modeling and understanding strongly correlated systems.

The impact of the summer School has been to expose to the listeners some of this richness, and to stimulate their awareness of each other's work, of the wide range experimental and theoretical tools and concepts, and of the proverbial "big picture."

Below, for completeness, is the conference photograph:

<u>Programme</u>

The schedule of the meeting was as following:

Sunday, July 25: arrival

Time	**Monday July 26**	**Tuesday July 27**	**Wednesday July 28**	**Thursday July 29**	**Friday July 30**
8.45-9.00	Welcome				
9:00-10.00	de Heer	Bohigas	Raizen	v. Issendorff	Reimann
10:00-11.00	Gaudefroy/Obertelli	v. Ruitenbeek	Guet	Ernst	Hansen
11.00-11.30	break	break	break	break	break
11:30-12:30	Benedek	Guet	Bohigas	Raizen	v. Issendorff
12:30-16:00	lunch free time	lunch free time	lunch	lunch free time	lunch free time
16:00-17.00	v. Ruitenbeek	Benedek	[*dep. 14:00*] Excursion to Selinunte	Reimann	Ernst
17.00-17.30	posters 1	break		posters 2	break
17:30-18:30		de Heer			Hansen
18:30-19:30		Obertelli/Gaudefroy			Kresin
20.00	dinner	dinner	dinner at Marinella	dinner	Banquet

Saturday, July 31: departure

As mentioned above, the listeners presented twenty-four posters.

Below are the abstracts of the invited lectures (in alphabetical order).

Giorgio Benedek
Shell effects in helium droplets
The diffraction experiments with helium droplets and their optical spectroscopy developed by J.P. Toennies *et al.* represent a breakthrough in the physics of finite atomic quantum systems. These experiments have unveiled the existence of magic numbers in bosonic clusters, the occurrence of resonant long-living collective excitations in ^{3}He and mixed ^{3}He/^{4}He droplets, the onset of superfluidity in ^{4}He clusters of a few atoms, and other intriguing phenomena. Magic numbers in ^{4}He clusters as well as zero-sound resonances in doped ^{3}He and mixed droplets are here presented as further examples of shell effects in finite quantum systems.
The first lecture describes Toennies *et al.* experiments where helium droplet beams are produced by vacuum expansion of the liquid. Illustration is given of the physical bases of the droplet number spectroscopy by diffraction experiments and of the optical spectroscopy of their elementary excitations through the insertion of chromophore probes. The observation of magic numbers in ^{4}He clusters will be analyzed and explained in terms of Auger evaporation processes.
The second lecture illustrates the experimental observations of shell excitations in doped ^{4}He, ^{3}He and mixed ^{3}He^{4}He droplets. The onset of superfluidity in mixed droplets as a function of the ^{4}He atom number is analyzed through the evolution of the collective excitations and the appearance of the rotonic peak. This analysis is then extended to the beautiful experiments by Stienkemeier, Ernst, Scoles and Higgins on the optical spectroscopy of alkali atoms and dimers floating of the droplet surface, which are shown to carry information on droplet surface collective excitations.

Oriol Bohigas
The compound nucleus, random matrix theories and chaotic dynamics
In studying nuclear properties, N.Bohr put forward the concept of the compound nucleus in the early 1930's. Trying to have an organizing principle in the statistical description of the compound nucleus resonances, Wigner introduced in physics in the early 1950's ensembles of random matrices, inspired

by work done earlier by statisticians. A remarkable consistency between random matrix theory predictions and observations has since then been established. One possible explanation of the success of the theory has emerged in the last twenty years: there exist universality properties of quantum fluctuations for systems whose classical analogue is chaotic (quantum chaos). Two seemingly disconnected fields, namely random matrices and chaotic dynamics, have therefore been related. Surprisingly, this connection has also a number of theoretical analogues (Riemann's zeta function). In the first lecture (Random Matrix Theories), the concept of the compound nucleus, the observation of its resonances and the random matrix modeling, as well as some results, will be discussed. In the second (Chaotic Dynamics) some basics as well as the main ingredients of periodic orbit theory, in discussing quantum systems, will be treated. The output will be a link between random matrix theories and chaotic dynamics.

Wolfgang Ernst

Shell models for alkali metal trimers: Electronic level structure and magnetic properties

Alkali metal trimers are produced in their low-spin (doublet) state configuration in molecular beams and in their high-spin (quartet) state configuration on cold helium droplets. Using laser spectroscopic methods, we investigate electronic ground and excited states and compare the results with our own quantum chemical calculations. Magnetic field measurements provide insight into spin-orbit and vibronic coupling effects. As result, we find that the electronic level structure of low-spin potassium and rubidium trimers is in good agreement with the classical shell model as it was developed 20 years ago for Na_3. In the high-spin configuration with three unpaired electrons of parallel spin, the level structure is significantly different and turns out to be related to the eigenstates of the harmonic oscillator, a feature known from the description of single-particle states in quantum dots.

Laurent Gaudefroy and Alexandre Obertelli

Developments in shell effect description of nuclear structure

Atomic nuclei are finite systems composed of fermions, the nucleons, and essentially governed by the strong interaction and quantum mechanical laws. Their structure is characterized by single-particle orbitals grouped in energy shells, separated by energy gaps leading to the so-called "magic numbers" of nucleons. Model describing the atomic nucleus have been built from the knowledge on stable nuclei. Important developments in radioactive beams and detection systems during the past 30 years help increasing the quantity and quality of the experimental data obtained on unstable nuclei, leading to a refined description of nuclear structure. (i) The major shells observed for stable nuclei evolve for neutron-rich nuclei and might disappear while new magic numbers of nucleons may arise. (ii) The shell structure in light radioactive nuclei can give rise to exotic phenomena such as neutron halos or clusters. (iii) In deformed nuclei, different shapes may compete for the ground state wave function. In some regions of the nuclear landscape, nuclei experience shape coexistence with a ground state being a superposition of different intrinsic deformations. (iv) The existence of super-heavy elements is only due to the quantum nature of nuclei and shell structure. These lectures aim at providing an overview of recent major achievements in these manifestations of shell effects in atomic nuclei.

Claude Guet

Linear and non-linear electron dynamics in finite systems

Surface plasmons in metallic nanoparticles
Red shifts and anharmonicities. Separation of center-of-mass and intrinsic excitations
Alternative model based on variational RPA
Semi-classical TDDFT
Plasmon relaxation
Coupled dynamics of electrons and ions in nanoparticles induced by short laser pulses
Finite size effects on the optical properties of dense plasmas

Klavs Hansen

Thermodynamics of finite systems

Finite systems have several properties that set them apart from macroscopic systems of similar composition. Some of these difference are due to the finite and often small heat capacity, and others are caused by quantum size effects that will influence the excitation spectrum. Finite sizes will also be manifested very strongly in studies of microcanonical ensembles, as for example used in molecular beam experiments.

The lectures will consist of two parts. In the first, the quantum size effects will be illustrated in detail with results on the thermodynamics of the shell structure of valence electrons in simple metal clusters. The second part will treat the melting of rare gas clusters that are ordered into packing shell and will include numerical simulations that illustrate the concept of microcanonical temperature, negative heat capacities etc.

Walt de Heer

Fundamentals of electronic shell structure in alkali clusters: Experiments and concepts

A short review of the development of the shell structure concepts in small alkali cluster will be presented with historical notes. Experimental aspects and basic theoretical concepts will be addressed

Bernd von Issendorff

Photoelectron spectroscopy of nanoclusters

Principles of energy- and angle-resolved photoelectron spectroscopy of the electronic structure of nanoclusters. Angular momenta and shape effects, and "crystal field" perturbations.

Vitaly Kresin

Long-range polarization interactions

Systems with high electric polarizabilities, such as metal nanoclusters and Rydberg atoms, can experience strong long-range forces. I will give an overview of some phenomena in which polarization interactions play a critical role. These phenomena include capture and emission of electrons and ions, surface scattering, cluster fission, and dispersion (London-van der Waals) forces.

Mark Raizen

Comprehensive control of atomic motion

The method of laser cooling has opened the door to low temperature physics of dilute gases. Despite the great success of this method, it has been limited to a very small set of atoms in the periodic table. I will describe in this talk new approaches to trapping and cooling that have been developed in my group. The first step uses pulsed magnetic fields to stop atoms and molecules where they can be magnetically trapped. The next step is an experimental realization of informational cooling as first proposed by Leo Szilard in 1929 in an effort to resolve the paradox of Maxwell's demon. Together, these provide a two-step comprehensive solution to trapping and cooling. I will describe our progress in applying these methods to controlled deposition of atoms on a surface. This will be a "bottom-up" approach to building complexity of finite quantum systems.

Stephanie Reimann

Shells and spins in quantum dots, and from quantum dots to cold atoms

The first lecture will focus on shell structure in vertical as well as lateral dots; quantum dots in quantum wires; transport and related issues of quantum Hall physics; and related systems.

The second lecture will highlight the many analogies between finite boson and fermion systems, and also comment on the fascinating aspects of the newly emerging research field of "atomtronics".

Jan van Ruitenbeek

Shell structure in metallic nanowires

Lecture 1. Introduction to metallic nanowires. Summary of the experimental techniques. The concept of conductance quantization and the realization in real metallic wires. Methods for analyzing conductance channels. Chains of metal atoms.

Lecture 2. Shell structure in free-electron like metallic nanowires. Review of the experimental evidence and the theoretical concepts. Supershell structure. Crossover to atomic (geometric) shell structure.