

Shell Effects in Finite Quantum Systems

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International School of Solid State Physics (50th Course) at the Ettore Majorana Centre for Scientific Culture

Overview of planned lectures (in alphabetical order)

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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 ^3He and mixed $^3\text{He}/^4\text{He}$ droplets, the onset of superfluidity in ^4He clusters of a few atoms, and other intriguing phenomena. Magic numbers in ^4He clusters as well as zero-sound resonances in doped ^3He 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 ^4He clusters will be analyzed and explained in terms of Auger evaporation processes.

The second lecture illustrates the experimental observations of shell excitations in doped ^4He , ^3He and mixed $^3\text{He}/^4\text{He}$ droplets. The onset of superfluidity in mixed droplets as a function of the ^4He 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 differences 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.