Quantum shell structure in metal clusters

This talk concerns the properties and significance of shell structures, particularly in metal clusters. We shall start by considering the general phenomenon of shell structures.

Electrons on isolated atoms reside in distinct *shells*, each with different energy and maximal occupation. The occupations are 2, 10, 18 and so on. A closely related set of "magic numbers" exists for protons and neutrons forming the atomic nucleus. In either case the occupation of the outer shell largely determines stability.

More recently, clusters of atoms have been observed[1] to exhibit similar sets of magic numbers. This behaviour can be observed even for clusters larger than a thousand atoms. Semiclassical theory[2] predicts electronic trajectories riminiscent of those in the Bohr atomic model, but with polygonal shapes. It turns out that the properties of these trajectories explain the observed shell structure and corresponding magic numbers. Depending on the cluster size, the phenomenon can have profound effects on catalytic properties, the exploration of which is an ongoing project.

References

[1] J. Pedersen, S. Bjrnholm, J. Borggreen, K. Hansen, T. P. Martin, H. D. Rasmussen: *Observation of quantum supershells in clusters of sodium atoms*. Nature **353**, 733-735 (1991).

[2] R. Balian and C. Bloch: *Distribution of Eigenfrequencies for the Wave Equation in a Finite Domain: III. Eigenfrequency Density Oscillations*. Ann. Phys. **69**, 76-160 (1972).