Fizički odsjek Prirodoslovno matematičkog fakulteta Sveučilišta u Zagrebu
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Seminar Fizičkog odsjeka

Vrijeme (s.t.)	Mjesto
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Wigner Crystallization in Central Potentials

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In 1934, Eugene Wigner predicted spatial localization of electrons in a low- density homogeneous electron gas (HEG). This Wigner crystallization, which is triggered when the kinetic energy of HEG is sufficiently small relative to the sum of the electron-electron repulsion energy and the energy of interaction of electrons with the uniform neutralizing background, is sudden i.e. it is associated with crossing of two energy levels. In 3D, HEG crystallizes at the Wigner-Seitz radius $r_s = 106$ (in atomic units), producing the body-centered cubic lattice, whereas in 2D the Wigner crystallization takes place at $r_s = 31$, the resulting lattice being hexagonal (triangular).

In general, weak confinement is a prerequisite for formation of the Wigner crystals, which are simply classical systems perturbed by zero-point vibrations about equilibrium positions of the constituting particles. In ground states of fully Coulombic systems (i.e. atoms and molecules), autoionization precludes Wigner crystallization. However, systems with unbound confining potentials (e.g. harmonium atoms) crystallize gradually upon decrease of the confinement strength.

In this talk, several aspects of Wigner crystallization in central confining potentials are discussed. In particular, the following subjects are covered:

1. Harmonium atoms and their weak- and strong-correlation limits.
2. Robust interpolation between the weak- and strong-correlation limits.
3. Correlation in Coulomb crystals: the Madelung energy and its variational estimation.
4. Smooth, oscillatory, and fluctuating components of energies of Coulomb crystals.
5. The ground-and excited-state wavefunctions at the strong-correlation limit.
6. The corresponding 1-matrices, natural spinorbitals, and their occupancies.

Voditelji seminara FO

Damir Pajić i Ivica Smolić