Kolokvij Grupe za računalne bioznanosti i Sekcije za teorijsku i računalnu kemiju Hrvatskog kemijskog društva

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Friday, October 4, 2019
III Wing lecture hall
11:00 - 12:00 pm

DENSITY OSCILLATIONS OF ONE-DIMENSIONAL CORRELATED ELECTRON SYSTEMS FROM DENSITY FUNCTIONAL THEORY

Gapless quasi-one-dimensional systems are not described by Fermi liquid theory, as is the case of interacting systems in higher dimensions, but rather by another unique framework, the Luttinger liquid theory. Our work is focused on the questions regarding strongly correlated one-dimensional Luttinger liquid physics. In particular, we try to bridge the gap between what is known from field theoretical methods, such as bosonization, and the real physical systems that are fabricated in the laboratory. Beyond weak interactions this gap is wider than most theorist imagine and experimentalist would like.

By starting from microscopic models we investigate, whether or not, methods such as Kohn-Sham Density Functional Theory (KS DFT) using the Local Density Approximation (LDA) for the exchange-correlation potential can lead to a correct description of the underlying Luttinger liquid low-energy fixed point. Basic theorems of KS DFT guarantee that the KS ground state charge density matches the density of the fully interacting many-body system if the exchange-correlation potential is exact. Therefore, in our work, we focus exclusively on the oscillations, known as Friedel oscillation, that occur in the density in presence of a boundary (or infinitely strong impurity). The power-law decay of the Friedel oscillations, away from the boundary and into the bulk, represent one of the hallmarks of the Luttinger liquid paradigm. In particular, we use the Hartree-Fock approximation to investigate the power-law decay of Friedel oscillations, propose a method to compute the density based on Matsubara Green's functions and most importantly clarify the limitations of LDA in describing Luttinger liquids.