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JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Seminar über Quanten-, Atom- und Neutronenphysik (QUANTUM)

Jan. 31, 2019 at 2 p.m. c.t.
Lorentz-Raum (05-127), Staudingerweg 7

Note: Vortrag im Rahmen des SFB/TR 49-Kolloquiums

Prof. Dr. Maurits W. Haverkort
Institute for Theoretical Physics, Heidelberg University

Correlations and multiplets; nuclear decay, exotic ordering in solids, and active transition metal centers in enzymes

Non-trivial electronic correlations and entanglement turn the prediction of many physical and chemical phenomena into a hard problem. The exponential scaling of the Hilbert space with system size eludes a direct solution of the Schrdinger (Dirac) equations. For the prediction of about 1/3 of all phenomena and materials, mean-field theory (Hartree-Fock or Density functional theory in the local density approximation) gives a reasonable result. When mean-field theory fails the discrepancy to reality can be so sever that one is not able to give a qualitative correct picture. Predicting, for example, if paramagnetic NiO is a metal or an insulator is still an open problem.

Using a combination of Quantum chemistry methods (RAS-CI) and renormalisation group theory we show how local correlations can be treated and influence material properties. Multiplets give rise to new low lying excitations in transition metal complexes important for many catalytic reactions and active centers of enzymes. Electronic interactions in 163Ho give rise to core electron multiplets that change the nuclear decay probability due to electron capture as a function of the energy of the additional neutrino that escapes. In several solids local interactions give rise to low energy

degrees of freedom that can lead to ordering, from conventional magnetic ordering in NiO to hidden order in URu2Si2, whose nature is still a mystery despite 30 years of research.

Local interactions are important, but it is the interaction of these localised states either with themselves on a lattice, or with a continuum, that makes our world so interesting. Using diagrammatic methods, starting with a bare Green's function that includes all local many-body interactions, we show how at least part of these effects can be treated.

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