凝縮系物理学ゼミナール
Condensed Matter Seminar

Location: Room 413, School of Science Bldg. 5 (理学 5 号館 413 号室)
Date: 13:30-15:00, Wednesday, 6 November 2013

“Density-matrix functionals from Green's functions”

Speaker: Prof. Dr. **Thomas Pruschke**
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Abstract:
The exact reduced density-matrix functional is derived from the Luttinger-Ward functional of the single-particle Green's function. Thereby, a formal link is provided between diagrammatic many body approaches using Green's functions on the one hand and theories based on many-body wave functions on the other. This link can be used to explicitly construct approximations for the density matrix functional that are equivalent with standard diagrammatic re-summation techniques and with non-perturbative dynamical mean-field theory in particular. Contrary to functionals of the Green's function, the exact density-matrix functional is convex and thus provides a true minimum principle which facilitates the calculation of the grand potential and derived equilibrium properties. The benefits of the proposed Green's-function-based density-matrix functional theory for geometrical structure optimization of strongly correlated materials are discussed.