UNIVERSITY OF GOTHENBURG

Periodized Thermal Greens Functions and Applications

Andro Sabashvili

Thesis for the defence of the degree of Doctor of Philosophy in Physics at the University of Gothenburg. The thesis will be presented on September 23, at 10:00 in KB, Chalmers Campus Johanneberg, Kemigården 4.
The presentation will be in english.

Opponent: Prof. André-Marie Tremblay
Department of Physics, University of Sherbrooke
Canada

Examiner: Prof. Henrik Johannesson

Supervisor: Prof. Stellan Östlund

Periodized Thermal Greens Functions and Applications

Andro Sabashvili

Department of Physics
University of Gothenburg
SE-412 96 Göteborg, Sweden

Abstract

This work describes a new formalism for Fermionic thermal Greens functions that are discretized in imaginary time. The discretization makes the thermal Greens function periodic in imaginary (Matsubara) frequency space and requires a generalisation of the Dyson equation and Luttinger-Ward-Baym-Kadanoff functional. A Padé method is used to perform an analytic continuation of the periodized Matsubara Greens function to real frequencies which conserves the spectral weight and thus the discontinuity of the corresponding real time Greens function at $t = 0$. Due to the Matsubara Greens function periodicity, the discrete imaginary frequency space is relatively small which allows calculations at the extremely high precision which is necessary to perform a reliable Padé fit. We use the method to compute the single particle spectral function and energy loss function for doped bilayer graphene in the two-band limit, described by parabolic dispersion and Coulomb interaction. Calculations are performed in both the random phase approximation (RPA) and the fully self-consistent GW approximation. The formalism is also applied to dynamical mean field theory calculations using iterated perturbation theory (IPT) for the paramagnetic Hubbard model.