Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Improved Description of Electron-Plasmon Coupling In Green's Function Calculations[1] JIANQIANG ZHOU, LUCIA REINING, Laboratoire des Solides Irradies, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France. European Theoretical Spectroscopy Facility (ETSF) — Green's function (GF) methods have been very successful for describing one- or two-particle excitations in solids. The GW approximation [1] is a well established approach for describing quasi-particle peaks in the spectral function. Beyond GW, the cumulant expansion, which is based on a hole-boson coupling model, gives a better description of plasmon satellites [2,3]. However, this traditional time-ordered cumulant (TOC) is only valid far from the Fermi level. Recent development [4] of a generalized cumulant (GC) improves the spectral function close to the Fermi level, but a framework for systematically improving is still missing. Here we show how GW, TOC and GC can be derived as a successive series of approximations in a unified way, and how one can go beyond today's state-of-the-art methods. Results for spectral functions and total energies of an exactly solvable model show that systematic improvement is obtained.

[1] L. Hedin, Phys. Rev. 139 A796 (1965).
[2] F. Aryasetiawan, L. Hedin and K. Karlsson, Phys. Rev. Lett. 77 112268 (1996).
[3] M. Guzzo et al, Phys. Rev. Lett. 107 166401 (2011).
[4] J. J. Kas, J. J. Rehr, and L. Reining, Phys. Rev. B 90 085112 (2014).

[1]Work supported by FP7/ERC Grant Agreement n. 320971

Jianqiang Zhou
Laboratoire des Solides Irradies, Ecole Polytechnique,
CNRS-CEA/DSM, F-91128 Palaiseau, France

Date submitted: 14 Nov 2014 Electronic form version 1.4