

MAR16-2015-005079

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

A direct approach to the calculation of many-body Green's functions: quasi-particles and more¹

LUCIA REINING, CNRS-Ecole Polytechnique

Many-body perturbation theory is a powerful approach to describe many properties of materials. Most often one uses Dyson equations with self-energy kernels that are approximated to low order in the interaction. In Hedin's GW approximation, for example, the self-energy is a product of the one-body Green's function and the screened Coulomb interaction. This is the state-of-the art method for bandstructure calculations in a wide range of materials. However, sometimes the GW approximation and related approaches are not sufficient, for example when one is interested in satellite structure beyond the quasi-particle peaks in the spectral function, or in the case of strong coupling, where the quasi-particle picture is no longer adequate. We explore an alternative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-body Greens function to its functional derivative with respect to an external perturbing potential [1]. This set of equations can be used to generate the perturbation series. Here we will show that working directly with the differential equations yields precious insight concerning some fundamental questions, guidelines for practical calculations, and methods that lead to an improved description of spectra, in particular advanced versions of the cumulant expansion. Results will be illustrated on various levels of approximation starting from simple models [2], but with a focus on full ab initio calculations [3] and comparison with, and interpretation of, experiment. In particular, we will discuss various kinds of photoemission satellites, and also address questions linked to strong correlation. [1] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (New York: Benjamin, 1962) [2] A. Stan et al., New J. Phys. 17, 093045 (2015) [3] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011); Phys. Rev. B 89, 085425 (2014)

¹This work has been carried out in collaboration with colleagues in the European Theoretical Spectroscopy Facility