Photoemission Spectra beyond GW : the Band Gap in Strongly Correlated Systems

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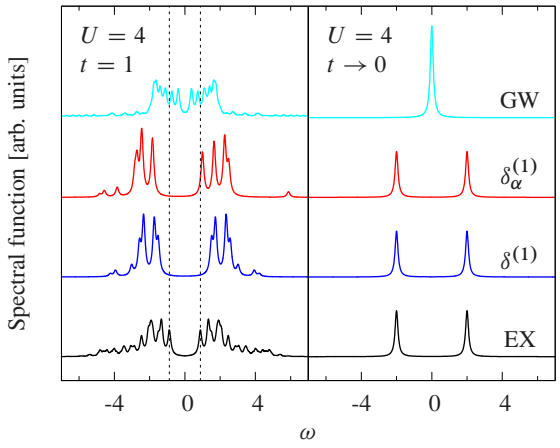

FIGURE 1: Spectral function for a 12-site Hubbard ring at 1/2 filling : exact (EX) *vs* MEET with exact one- and two-body RDMs ($\delta^{(1)}$), MEET with approximate one- and two-body RDMs ($\delta^{(1)}_\alpha$), and *GW* method.

Photoemission is a powerful tool to obtain insight into the electronic structure and excitations in materials. From the theoretical point of view Many-Body Perturbation Theory, within the so called GW approximation to electron correlation, is the method of choice for calculations of photoemission spectra of many materials. However GW suffers from some fundamental shortcomings, and, in particular, it does not capture strong correlation, unless one treats the system in a magnetically ordered phase. In this talk we present various efforts to go beyond *GW* [1-3]. In particular, we focus on a many-body effective-energy theory (MEET) that gives many-body spectral functions in terms of reduced density matrices (RDMs) [4]. We show that simple approximations, which require the knowledge of the lowest *n*-body RDMs only, can provide accurate photoemission spectra in model systems in the weak as well as strong correlation regime. With the example of bulk NiO, we show that our method yields a qualitatively correct picture both in the antiferromagnetic and paramagnetic phases, contrary to mean-field methods, in which the paramagnet is a metal.

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[2] P. Romaniello, F. Bechstedt, and L. Reining, Phys. Rev. B 85, 155131 (2012)
[3] G. Lani, P. Romaniello, and L. Reining, New J. Phys. 14, 013056 (2012)
[4] S. Di Sabatino, J.A. Berger, L. Reining, and P. Romaniello, under revision