

Abstract Submitted
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Applications of the Retarded Cumulant Expansion to Realistic Systems¹ J.J. KAS, J.J. REHR, U. Washington — The cumulant expansion of the one-electron Green's function has proved extremely useful in describing electron correlation in materials beyond the one-electron approximation.² For example, the approach improves on the GW approximation, accounting for multiple satellites in the spectral function and x-ray photoemission spectra. Previous implementations based on the time ordered representation ignore diagrams which lead to partial occupations and satellite features in the spectral function above and below the Fermi surface. Recently, we have shown that these difficulties can be overcome with a cumulant expansion of the retarded Green's function.³ This model was tested on the homogeneous electron gas, giving good results for the spectral function, correlation energies, and occupation numbers. In this follow-up, we discuss the extension of the approach to realistic condensed matter systems, using GW calculations of the self-energy to approximate the cumulant. Results are presented for the spectral function and occupation numbers, and compared to experimental XPS data.

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²Matteo Guzzo et al. Phys. Rev. Lett. **107**, 166401 (2011) and Phys. Rev. B **89**, 085425 (2014).

³J. J. Kas, J. J. Rehr, and L. Reining, Phys. Rev. B **90**, 085112 (2014).

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