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Generalized Cumulant Expansion for the One Electron Green's Function[1] J.J. KAS, J.J. REHR, U. Washington, L. REINING, École Polytechnique — The cumulant expansion has proved extremely useful in describing many-body excitations. For example, the approach rectifies the failure of the GW approximation to account for multiple satellites in x-ray photoemission spectra.[2] However, current implementations are inadequate since they ignore diagrams that lead to partial occupations and satellite features in the spectral function both above and below the Fermi surface. Here, we correct these limitations using a cumulant expansion of the retarded one-electron Green's function. At 2nd order in the effective boson couplings, the cumulant is proportional to the GW self-energy. Thus the cumulant method extends the GW Green's function without additional computational expense, and can therefore be used for complex systems. We test the approach on the homogeneous electron gas, and present results for a range of parameters that are physically relevant for condensed matter systems. The resulting spectral function is used for calculations of occupation numbers, quasiparticle properties, and correlation energies.

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[2]Matteo Guzzo, Giovanna Lani, Francesco Sottile, Pina Romaniello, Matteo Gatti, Joshua J. Kas, John J. Rehr, Mathieu G. Silly, Fausto Sirotti, and Lucia Reining, Phys. Rev. Lett. 107, 166401 (2011)

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