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Many-electron interactions and first-principles studies of spectral functions: spin multiplets and plasmon satellites in photoemission spectra[1]

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The photoemission spectrum of an interacting system is often simply thought to be qualitatively similar to the corresponding non-interacting system: interactions only cause a shift and a broadening of the quasiparticle peak and result in a transfer of spectral weight into an incoherent background. We discuss two cases where this simple quasiparticle picture of photoemission fails and interactions result in a more drastic, qualitative difference from the non-interacting system. For electronic systems with unfilled shells, the coupling of angular momenta results in a multiplet structure in the photoemission spectrum. We describe how accurate calculations of multiplet splittings are possible within the GW approximation and present results for several magnetic molecules and defects, such as the negatively charged nitrogen-vacancy defect (NV^-) center in diamond. We also discuss plasmon satellite structures in photoemission spectra. We show for bulk silicon and doped graphene that the *ab initio*GW approximation overestimates the quasiparticle-satellite separation significantly and falsely predicts a plasmaron excitation. By including significant vertex corrections via the *ab initio*GW+cumulant approximation, we improve the description of plasmon satellites and find good agreement with experimental photoemission spectra.

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