

GW in Magnetic and Nearly Magnetic Systems

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The electronic properties of materials are often sensitive to physics beyond that captured by the LDA or DFT. One famous example is the band-gap of semiconductors, which tends to be predicted poorly by LDA but is described much more reliably by GW self-energy approximations. The GW approximation accounts for non-locality of the self-energy and for the role of particle-hole pair fluctuations that screen electron-electron interactions dynamically. The predicted properties of many magnetic systems are also extremely sensitive to exchange-correlation approximations, as is evident for example Len Kleinman's work on extremely thin magnetic films. I will discuss the possibility of improving the description of some magnetic systems by using a generalized GW approximation that accounts for the role of spin-flip particle-hole pair fluctuations.