The effects of nonlocal self-energy on the electronic structure of correlated materials

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When calculating the electronic structure of correlated materials it is often assumed that the self-energy is local and the Hubbard U is static. How these two approximations influence the electronic structure remains to be investigated. Recently substantial progress in solving the impurity problem with frequency-dependent Hubbard U has been achieved. This new algorithm makes it possible to perform LDA+DMFT calculations using a dynamic Hubbard U, instead of a static one as in conventional calculations. This raises an important issue concerning the role of k-dependent self-energy which tends to widen the band width. The use of dynamic U might lead to an overestimate of band narrowing or mass enhancement.

To address the above issues, we perform accurate calculations on real materials within the GW approximation. As a test case we study specifically the electronic structure of $SrVO_3$ which is a narrow-band system with one d-electron in the vanadium t_{2g} band. The results indicate that k-dependent self-energy widens the band width significantly. We believe the results are general and will be directly relevant to electronic structure calculations. To include nonlocal self-energy, a combination of the GW approximation and the dynamical mean-field theory (DMFT) was proposed some years ago and may provide a realistic way of including k-dependent self-energy.

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