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Dynamical susceptibilities and spontaneous symmetry breaking with dynamical mean-field theory

Abstract:

Combination of dynamical mean-field theory (DMFT) with ab initio band structure methods provided quantitive description electronic correlations in real materials. With spontaneous symmetry breaking being one of the most prominent correlation effects, DMFT allows access to various physical observables across phase transitions driven by temperature or other external parameters. For practical as well as fundamental reasons DMFT calculations focused largely on oneparticle dynamics so far. In particular, the behavior of collective modes associated with spontaneous symmetry breaking has been unexplored with DMFT. Here we present a computational study of dynamical susceptibilities across excitonic condensation transition in two-band Hubbard model. We demonstrate that DMFT correctly captures the Goldstone modes associated with breaking of continuous symmetries and investigate the smooth evolution from gapped Goldstone mode to a truly amplitude Higgs mode when symmetry-breaking terms of increasing strength are added to the Hamiltonian. Specific to the excitonic condensation, we observe a quantitative change in the dynamical spin susceptibility at the transition, which may serve as the experimental probe of the condensate. I will also discuss the computational limitations and feasibility of the present approach to real materials.

Geffroy et al. arXiv:1808.08046