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Many-body effects in iron pnictides and chalcogenides – non-local vs dynamic origin of effective masses JAN M. TOMCZAK, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, MARK VAN SCHILFGAARDE, Department of Physics, Kings College London, Strand, London WC2R 2LS, UK, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — We apply the quasi-particle self-consistent GW (QSGW) approximation to some of the iron pnictide and chalcogenide superconductors. We compute Fermi surfaces and density of states, and find excellent agreement with experiment, substantially improving over standard band-structure methods. Analyzing the QSGW self-energy we discuss non-local and dynamic contributions to effective masses. We present evidence that these two contributions are mostly separable. Indeed the quasi-particle weight is found to be essentially independent of momentum. The main effect of non-locality is captured by the static but non-local QSGW effective potential. Moreover, these non-local self-energy corrections, absent in e.g. dynamical mean field theory (DMFT), can be relatively large. We show, on the other hand, that QSGW only partially accounts for dynamic renormalizations at low energies. These findings suggest that QSGW combined with DMFT will capture most of the many-body physics in the iron pnictides and chalcogenides.

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