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An ab initio many-body approach to understanding magnetism in the unconventional superconductor, FeSe[1] BRIAN BUSEMEYER, LUCAS WAGNER, University of Illinois at Urbana-Champaign Physics Department — We report on the progress of many-body ab initio fixed-node diffusion Monte Carlo (FM-DMC) calculations performed on the unconventional superconductor FeSe. The exact nature of the pairing mechanism in unconventional superconductors is still controversial; however, the fact that these materials demonstrate antiferromagnetism near the conditions necessary for superconductivity suggests some combination of lattice and magnetic interactions may be responsible. FN-DMC has been shown to obtain high accuracy on a number of strongly correlated materials, and so is particularly well-suited to study the correlations that give rise to superconductivity. We perform FN-DMC calculations on FeSe to determine the energetic orderings of the low-lying magnetic states, and investigate the dominant correlations between the single particle states. FeSe also demonstrates a pressure dependent transition temperatures, hence, we also investigate the pressure dependence of the energy and dominant correlations in the various magnetic states. We expect our results will shed light on the nature of magnetism in the iron-based superconductors, and possibly its relationship with superconductivity.

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