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An ab-initio Quantum Monte Carlo analysis of pressure and magnetism in the unconventional superconductor, FeSe[1] BRIAN BUSEMEYER, LUCAS K. WAGNER, University of Illinois, Urbana-Champaign Physics Deptartment — We report the results of many-body ab-initio fixed-node diffusion Monte Carlo calculations performed on the unconventional superconductor, FeSe. FeSe shows a strong pressure-dependent critical temperature, and because magnetism is generally expected to play an important role in understanding unconventional superconductivity, for pressures ranging from ambient to 11 GPa, we investigate the single and many-body properties of three ordered magnetic configurations, including the two found in similar iron-based superconductors. Our calculations find that at least two magnetic orders (collinear and bicollinear) are nearly degenerate in energy, becoming closer in energy as pressure increases. We also analyze how correlations between the electrons change as a function of pressure, and discuss what this could mean for superconductivity.

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