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Effect of nodal surface on the geometry of antiferromagnetic iron oxide

Joshua P. Townsend, Luke Shulenburger, and Thomas R. Mattsson
Sandia National Laboratories, Albuquerque, NM 87185

Ken Esler
Stone Ridge Technology, Bel Air, MD 21015

Ronald E. Cohen
Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015

Abstract

We report quantum variational and diffusion Monte Carlo calculations of antiferromagnetic iron oxide (FeO) which offer a test of the accuracy and predictive power of a single slater-jastrow determinant representation of a highly correlated many-body wave function. We find that QMC predictions of the equilibrium rhombohedral distortion of the AFM B1 lattice at ambient density are highly sensitive to the construction of the QMC trial wave function and its nodal surface. The results highlight the need for more advanced descriptions of the many-body wave function required to obtain highly accurate properties strongly correlated systems within QMC.

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