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Magnetic properties and pairing tendencies of the iron-based superconducting ladder BaFe2S3:Combined ab-initio and density matrix renormalization group study NIRAVKUMAR PATEL, The University of Tennessee, ALBERTO NOCERA, GONZALO ALVAREZ, Oak Ridge National Laboratory, RYOTARO ARITA, RIKEN Center for Emergent Matter Science, ADRIANA MOREO, ELBIO DAGOTTO, The University of Tennessee — The recent discovery of superconductivity in the two-leg ladder compound BaFe2S3[1] opens a broad avenue of research, because it represents the first report of pairing tendencies in a quasi-one-dimensional iron-based high-critical-temperature superconductor. As in the case of the cuprates, ladders and chains can be far more accurately studied using many-body techniques and model Hamiltonians than their layered counterparts. We study a two-orbital Hubbard model derived from first principles that describes individual ladders of BaFe2S3using density matrix renormalization group [2]. Two main results are found: (i)at half-filling, ferromagnetic (antiferromagnetic) order emerges as the dominant magnetic pattern along the rungs (legs) of the ladder, in excellent agreement with neutron experiments; and (ii)with hole doping, pairs form in the strong coupling regime, as found by studying the binding energy. In addition, we also find binding tendencies in 1D chain of two-orbitals where the pair-pair correlations show inter-orbital singlet pairs on the neighboring sites. [1] H. Takahashi et al., Nat. Mater. 14, 1008(2015) [2] N. D. Patel et al., Phys. Rev. B 94, 075119 (2016)

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