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Numerical Study of a Multiorbital Hubbard Model for the Two-Leg Ladder $BaFe_2S_3$ High-Tc Superconductor Using the Density Matrix Renormalization Group NIRAVKUMAR PATEL, The University of Tennessee, Knoxville, Tennessee 37996, USA, ALBERTO NOCERA, GONZALO AL-VAREZ, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, RY-OTARO ARITA, RIKEN, 2-12-1 Hirosawa, Wako, Saitama 351-0198, Japan, ELBIO DAGOTTO, The University of Tennessee, Knoxville, Tennessee 37996, USA — Iron based high-Tc superconductors have attracted considerable attention because of its unconventional superconducting properties. Here, we analyze the magnetic and pairing characteristics of the recently discovered two-leg ladder material $BaFe_2S_3$ that becomes superconducting by applying pressure [1], using a two-orbital Hubbard model studied via the Density Matrix Renormalization Group technique. The hopping parameters, which spans up-to the 2^{nd} nearest-neighbor rungs, were obtained from the ab-initio downfolded band structure at ambient and high pressures [2]. The magnetic phase diagram at a realistic Hund coupling J/U = 0.25 is presented varying the Hubbard U, at select values of the electronic fillings. At half-filling, we find a robust magnetic order in excellent agreement with experiments [1] i.e. antiferromagnetic (ferromagnetic) along the leg (rung) directions. We also discuss a possible tendency for this system to form a paired bound state of holes in a small but finite window of Hubbard U. The symmetries of this tentative paired ground state will be discussed.

[1] Hiroki Takahashi et al., Nature Materials 14, 1008 (2015)

[2] Ryotaro Arita et al., Phys. Rev. B 92, 054515 (2015)

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