

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Verwey Metal-Insulator Transition in Magnetite from the Slave-Boson Approach** MOHAMMAD SHERAFATI, SASHI SATPATHY, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri, USA, DIX PETTEY, Department of Mathematics, University of Missouri, Columbia, Missouri, USA — We study the Verwey metal-insulator transition in magnetite (Ref.1) by solving a three-band extended Hubbard Hamiltonian for spinless fermions using the slave-boson approach, which also includes coupling to the local phonon modes. This model is suggested from the earlier density-functional studies of magnetite.(Ref.2) We first solve the 1D Hubbard model for the spinless fermions with nearest-neighbor interaction by both Gutzwiller variational and slave-boson methods and show that these two approaches yield different results unlike in the case of the standard Hubbard model, thereby clarifying some of the discrepancies in the literature (Ref.3), then we extend the formalism to three-band Hamiltonian for magnetite. The results suggest a metal-insulator transition at a critical value for the intersite interaction.

References:

- 1) E.J.W. Verwey, Nature 144, 327 (1939)
- 2) Z. Zhang and S. Satpathy, Phys. Rev. B 44, 13319 (1991)
- 3) P. Fazekas, Solid State Communications 10, 175 (1972); Physica Scripta, T29, 125 (1989); G. Seibold and E. Sigmund, Z. Phys. B 101, 405 (1996)

Mohammad Sherafati  
Department of Physics and Astronomy, University of Missouri, Columbia

Date submitted: 09 Nov 2012

Electronic form version 1.4