

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Theory of the magnetic and metal-insulator transitions in RNiO<sub>3</sub> bulk and layered**<sup>1</sup> BAYO LAU, ANDREW J. MILLIS, Department of Physics, Columbia University — A slave rotor-Hartree Fock formalism is presented for studying the properties of the p-d model describing perovskite transition metal oxides, and a flexible and efficient numerical formalism is developed for its solution. The methodology is shown to yield, within an unified formulation, the significant aspects of the rare earth nickelate phase diagram, including the paramagnetic metal state observed for the LaNiO<sub>3</sub> and the correct ground-state magnetic order of insulating compounds. It is then used to elucidate ground state changes occurring as morphology is varied from bulk to strained and un-strained thin-film form. For ultrathin films, epitaxial strain and charge-transfer to the apical out-of-plane oxygen sites are shown to have significant impact on the phase diagram.

<sup>1</sup>This effort is supported by US National Science Foundation under grant NSF-DMR-1006282

Bayo Lau  
Department of Physics, Columbia University

Date submitted: 09 Nov 2012

Electronic form version 1.4