Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Localized and itinerant magnetic excitations in $CaFe_2As_2$ LIQIN KE, MARK VAN SCHILFGAARDE, School of Materials, Arizona State University, VLADIMIR ANTROPOV, Condensed Matter Physics, Ames Laboratory, IA 50011, TAKAO KOTANI, Department of Applied Mathematics and Physics, Tottori University, Japan — Elementary magnetic excitations in the striped phase of $CaFe_2As_2$ are studied with linear-response density-functional theory. Itinerant, Stoner-like elementary excitations are found to coexist with the usual antiferromagnetic spin waves observed in neutron experiments. When the Fe moment M exceed $1.1\mu_B$, spin waves are dominant; while as M decreases below $1\mu_B$ there is a rather sharp transition to itinerant behavior, with spin waves being damped by Stoner excitations of several types. An unusual low energy excitation was found, whose origin can be traced to excitations within a narrow Fe d band of xy and yz symmetry. This band lies above the Fermi level when M is $1.1\mu_B$, and passes through it as M decreases. The more conventional spin waves are associated with transitions from a different band of d states, at lower energy. This establishes that independent localized and itinerant elementary excitations coexist in $CaFe_2As_2$, and are present even below the Néel temperature.

Liqin Ke
School of Materials, Arizona State University

Date submitted: 16 Dec 2009 Electronic form version 1.4