Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

The Truncated Polynomial Expansion Monte Carlo Algorithm for Spin-fermion Models: Application to Diluted Magnetic Semiconductors and Manganites CENGIZ SEN, Florida State University and National High Magnetic Field Laboratory, GONZALO ALVAREZ, Oak Ridge National Laboratory, ELBIO DAGOTTO, University of Tennessee and Oak Ridge National Laboratory — A system of fermions coupled to classical fields is common to a wide range of strongly correlated electron problems where the fermionic operators appear in the Hamiltonian involving only quadratic terms. A conventional approach to solve these kinds of models is by diagonalizing the fermions in the one-electron sector at finite temperature for a given configuration of classical fields. However, this results in a high computational cost as the computational complexity grows with the 4-th power of the size of the system. The Truncated Polynomial Expansion Monte Carlo Algorithm (TPEM), developed by N. Furukawa and Y. Motome (J. Phys. Soc. Jpn. **73**, (2004) 1482), replaces the exact diagonalization of the one-electron sector in these models and has a complexity that is linear with the size of the system. In this talk, I will discuss the performance and reliability of the method as well as the parallelization of the algorithm. I will also show novel applications of the TPEM to disordered systems in the context of diluted magnetic semiconductors and to finite Hund coupling models for manganites (G. Alvarez *et al.*, submitted to Computer Physics Communications). I will discuss how the TPEM can drastically improve the study of those systems.

Cengiz Sen
Florida State University and National High Magnetic Field Laboratory

Date submitted: 03 Dec 2004 Electronic form version 1.4