

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Implementing the  $SU(2)$  Symmetry for the DMRG<sup>1</sup>** GONZALO ALVAREZ, Oak Ridge National Laboratory — In the Density Matrix Renormalization Group (DMRG) algorithm (White, 1992), Hamiltonian symmetries play an important role. Using symmetries, the matrix representation of the Hamiltonian can be blocked. Diagonalizing each matrix block is more efficient than diagonalizing the original matrix. This talk will explain how the DMRG++ code<sup>2</sup> has been extended to handle the non-local  $SU(2)$  symmetry in a model independent way. Improvements in CPU times compared to runs with only local symmetries will be discussed for typical tight-binding models of strongly correlated electronic systems. The computational bottleneck of the algorithm, and the use of shared memory parallelization will also be addressed. Finally, a roadmap for future work on DMRG++ will be presented.

<sup>1</sup>Supported by the Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. Department of Energy, under contract with UT-Battelle.

<sup>2</sup>arXiv:0902.3185 or Computer Physics Communications **180** (2009) 1572-1578.

Gonzalo Alvarez  
Oak Ridge National Laboratory

Date submitted: 18 Nov 2009

Electronic form version 1.4