

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Finite-size correction in many-body electronic structure calculations of spin polarized systems**<sup>1</sup> FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, Department of Physics, The College of William and Mary — We extend the post-processing finite-size (FS) correction method, developed by Kwee, Zhang, and Krakauer<sup>2</sup>, to spin polarized systems. The method estimates the FS effects in many-body (MB) electronic structure calculations by a modified density functional theory (DFT) calculation, without having to repeat expensive MB simulations. We construct a unified FS DFT exchange-correlation functional for spin unpolarized and fully spin polarized systems, and then interpolate the results to arbitrary spin polarizations using the formula of Perdew and Wang<sup>3</sup> or that of Perdew and Zunger.<sup>4</sup> The application of this FS correction method to several typical magnetic systems with varying supercell sizes demonstrates that it consistently removes most of the FS errors, leading to rapid convergence of the MB results to the infinite size limit.

<sup>1</sup>Supported by DOE, NSF, ONR.

<sup>2</sup>H. Kwee, S. Zhang, and H. Krakauer, Phys. Rev. Lett. **100**, 126404 (2008)

<sup>3</sup>J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992)

<sup>4</sup>J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981)

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Date submitted: 29 Dec 2010

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