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Correction of Finite Size Errors in Many-body Electronic Structure Calculations[1] HENDRA KWEE, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — Finite-size (FS) effects are a major source of error in many-body (MB) electronic structure calculations of extended systems. Reducing FS errors is thus a key to broader applications of MB methods in real materials, and the subject has drawn considerable attention.[2] We show that MB FS effects can be effectively included in a modified local density approximation calculation. A parametrization for the FS exchange-correlation functional is obtained. The method is simple and gives post-processing corrections that can be applied to any MB results. Conceptually, it gives a consistent framework for relating FS effects in MB and DFT calculations, which is important if the two methods are to be seamlessly interfaced to bridge length scales. Applications to a model insulator (P_2 in a supercell), to semiconducting Si, and to metallic Na show that the method delivers greatly improved FS corrections.[3]

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[2]P. R. C. Kent *et. al.*, Phys. Rev. B **59**, 1917 (1999); S. Chiesa *et. al.* Phys. Rev. Lett. **97**, 076404 (2006).
[3]H. Kwee, S. Zhang and H. Krakauer (2007), preprint at http://arxiv.org/abs/0711.0921.

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