

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Efficient method of finite-size correction in quantum Monte Carlo calculations SAM AZADI, Department of Physics and Tomas Young Centre, University College London, MATTHEW FOULKES, Department of Physics, Imperial College London — We present a simple but efficient method of finite size correction for metallic crystals [1]. Our method is based on an accurate combination of twist averaging boundary condition and density functional theory. We compare our method with several previously introduced schemes. Our quantum Monte Carlo results for lithium and aluminium show the accuracy and practicality of our method. :1] Sam Azadi, and W. M. C. Foulkes, *J. Chem. Phys.* **143**, 102807 (2015).

Sam Azadi
Department of Physics and Tomas Young Centre, University College London

Date submitted: 01 Dec 2015

Electronic form version 1.4