Reciprocal space approach to finite size error in many-body simulations

SIMONE CHIESA, DAVID CEPERLEY, RICHARD MARTIN, University of Illinois at Urbana-Champaign, MARKUS HOLZMANN, Université P. et M. Curie, Paris, France — A scheme for the correction of the finite size error in the potential energy occurring in the quantum Monte Carlo simulation of the bulk materials is presented. It is based on the fact that the potential energy can be written as a sum over the static structure factor, \( S(k) \), and on the assumption that \( S(k) \) does not depend on the simulation cell size. The error in the potential energy is then an integration error and corrected by an improved integration scheme. This also leads to an understanding of the scaling of the error with system size. Applications to the electron gas and to a novel nitrogen structure are presented.