A theory of finite-size effects in periodic coupled cluster calculations

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Many body perturbation theory (MBPT) and coupled cluster (CC) theory have been successfully applied to molecular systems for decades. Properties of periodic systems need to be evaluated at the thermodynamic limit (TDL), and practical calculations therefore suffer from finite-size errors. Due to the singularity caused by the long range Coulomb interaction, the convergence of the energy and other physical properties towards the TDL is often slow and follows a low-order power law. It is therefore important to understand the precise finite-size scaling. Our approach interprets the finite-size error as a numerical quadrature error for certain singular and complex integrands. Assuming the Hartree-Fock orbitals and orbital energies can be exactly evaluated at any k-point, we will present a theory of finite-size effects in ground-state energy calculations of insulating systems using the simplest and representative CC theory, i.e., the coupled cluster doubles (CCD) theory. We will also discuss its implication in periodic MBPT calculations, and if time permits, strategies to reduce the finite-size error using certain staggered mesh methods.