Ab-initio electronic structure calculations of periodic systems in the presence of arbitrary magnetic fields

ALFREDO CORREA, LLNL, GIULIA GALLI, UC Davis, WEI CAI, Stanford University — Ab initio electronic structure calculations in the presence of magnetic fields have been mainly performed for isolated systems, or, in the case of periodic systems, by adopting perturbative approaches. Building on a recent formulation of electronic structure calculations in the presence of magnetic fields [1,2], we will discuss calculations for periodic systems under arbitrary conditions, which include arbitrary (finite) magnetic field, arbitrary periodic cell shapes, and magnetic field spatial variations. Preliminary results based on a planewave numerical approach and local approximations to Density Functional Theory will be presented.[1] W.Cai, G.Galli, Phys. Rev. Lett. 92, 186402 (2004).[2] E. Lee, W. Cai, G. Galli, J. Comput. Phys. 226, 1310 (2007)

1Prepared by LLNL under Contract DE-AC52-07NA27344 and SciDAC Grant DE-FC02-06ER46262.