Ab initio investigation of magnetic transport properties by Wannier interpolation

YUGUI YAO, Institute of Physics, CAS, Beijing 100190, China & Department of Physics, University of Texas, Austin, Texas 78712, USA, YI LIU, Institute of Physics, CAS, Beijing 100190, China — An efficient ab initio approach for the study of magnetic transport properties is developed based on the Boltzmann equation with the Wannier interpolation scheme. Using this method, we can investigate magnetoresistance [1], low field Hall coefficient, anomalous Hall effect, orbit magnetization, cyclotron motion and the effective mass, etc. As a typical application of this method, we present the band-resolved electric conductivities of MgB$_2$ under finite magnetic fields, multiband characters for the individual bands are revealed. Combined with experimental result, fully band resolved scattering rate for each band was obtained for MgB$_2$. It seems that the scattering from el-ph coupling or impurities affects the $\pi_1$ band more weakly [2].