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 π_1 band more weakly [2].

[1] Yi Liu, Hai-Jun Zhang, and Yugui Yao, Phys. Rev. B 79, 245123 (2009);
[2] H. Yang, et al. Phys. Rev. Lett 101, 067001 (2008).

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