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Perturbation energy as an alternative to the total energy calculations[1] ANDREY KUTEPOV, VLADIMIR ANTROPOV, Ames Laboratory, Ames, USA, MARK VAN SCHILFGAARDE, King's College, London, UK, VICTOR ANTONOV, Institue for Physics of Metals, Kiev, Ukraine — We analyze different approaches to determine the energy from a perturbation using modern electronic structure methods. We compare the energy of perturbation from standard perturbation theory with what is obtained directly in self consistent band structure methods. The method is applied for studies such perturbations as internal magnetic field and spin orbital coupling in solids. This method is further compared with integration over the coupling constant. Numerical tests have been performed for magnetic Fe and Gd systems using the local density approximation. The main advantage of present scheme is its usefulness in methods for strongly correlated electronic systems studies where total energy calculations are not always possible. Specific calculations are performed using self consistent quasiparticle GW and LDA+U calculations for MnBi where the right value of magnetic moment and sign/value of magnetic anisotropy as a function of temperature have been obtained.

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