

Abstract Submitted  
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**Density matrix perturbation theory for magneto-optical response of periodic insulators**<sup>1</sup> IRINA LEBEDEVA, ILYA TOKATLY, ANGEL RUBIO, Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del País Vasco, Spain — Density matrix perturbation theory offers an ideal theoretical framework for the description of response of solids to arbitrary electromagnetic fields. In particular, it allows to consider perturbations introduced by uniform electric and magnetic fields under periodic boundary conditions, though the corresponding potentials break the translational invariance of the Hamiltonian. We have implemented the density matrix perturbation theory in the open-source Octopus code on the basis of the efficient Sternheimer approach. The procedures for responses of different order to electromagnetic fields, including electric polarizability, orbital magnetic susceptibility and magneto-optical response, have been developed and tested by comparison with the results for finite systems and for wavefunction-based perturbation theory, which is already available in the code. Additional analysis of the orbital magneto-optical response is performed on the basis of analytical models. Symmetry limitations to observation of the magneto-optical response are discussed.

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Irina Lebedeva  
Universidad del País Vasco

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