Abstract Submitted
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Time-dependent density functional theory of magneto-optical response of periodic insulators[1] ANGEL RUBIO, Universidad del Pais Vasco, ILYA V. TOKATLY, IRINA V. LEBEDEVA, Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Universidad del Pais Vasco, Spain — Though the linear response theory has been successfully used for molecular systems for a long time, the extension of this theory to solids is not straightforward since the position operator is ill defined in extended periodic systems. The theoretical description of homogeneous static magnetic field in periodic systems is particularly challenging as the corresponding vector potential breaks the translational invariance of the Hamiltonian. We present a unified approach to calculation of all-order response to arbitrary electromagnetic fields both for periodic and molecular systems within the formalism of non-equilibrium Green functions. The approach is applied to derive the expression for the magneto-optical response of insulating solids in the approximation of non-interacting electrons. The formula obtained is completely identical to the expression for molecular systems if the proper position and orbital magnetization operators are chosen. The terms corresponding to changes in the optical response due to the orbital magnetization of Bloch states and due to the modified density of Bloch states in the magnetic field are identified. A computational scheme based on the density matrix-perturbation theory is developed for practical calculations of the magneto-optical response.

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