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Time-dependent density functional theory of magneto-optical response

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Though the perturbation theory has been successfully used to describe various types of responses of molecules to electromagnetic fields for a long time, the extension of this theory to solids is not straightforward since the position operator is ill defined for such systems. The theoretical description of
magnetic fields in periodic systems is particularly challenging as it leads to non-perturbative changes in eigenstates. We present an approach to calculation of magneto-optical response within the density matrix formalism applicable both to molecules and solids. The density matrix perturbation theory is implemented in open-source Octopus code using efficient Sternheimer method for solution of the Liouville equation. The implemented procedures are tested against available literature data for molecular and crystalline systems.

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