# Natural optical activity in solids: an *ab initio* approach based on Wannier interpolation

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When electromagnetic waves interact with a periodic solid, a number of interesting phenomena can take place, according to the symmetry properties of the system. Among them we mention, e.g., linear birefringence and dichroism, the Faraday effect, natural optical activity (rotatory power and circular dichroism), gyrotropic birefringence, and non-reciprocal dichroism. Such phenomena are encoded in the frequency- and momentum-dependent optical conductivity linear response $\sigma_{\alpha\beta}(\omega,\mathbf{q})$. Upon expansion in powers of the wave vector $\mathbf{q}$ of the incident light, $\sigma_{\alpha\beta}(\omega,\mathbf{q})$ reads

$$\sigma_{\alpha\beta}(\omega,\mathbf{q}) = \sigma^{(0)}_{\alpha\beta}(\omega) + \sigma_{\alpha\beta,\gamma}(\omega)\, q_\gamma + \mathcal{O}(q^2),$$

with a sum over $\gamma$ implied. The zeroth-order term $\sigma^{(0)}_{\alpha\beta}(\omega)$ describes linear birefringence and dichroism, as well as the Faraday effect, which are present even in centrosymmetric periodic solids. On the other hand, the first-order term $\sigma_{\alpha\beta,\gamma}(\omega)$ captures spatial-dispersive phenomena, such as natural optical activity in acentric non-magnetic materials, as well as gyrotropic birefringence and non-reciprocal dichroism in acentric antiferromagnets.

Recently, an approach for the calculation of the aforementioned spatial-dispersive optical conductivity, based on a Kubo-Greenwood formulation, has been proposed [1]. In this work, we present an implementation of this theoretical framework using Wannier interpolation. This technique is particularly well suited for treating interband optical transitions in small-gap semiconductors because these require a fine sampling in reciprocal space to obtain a well resolved spectrum, a requirement that is hard to meet with direct *ab initio* calculations. Furthermore, we test our implementation with some benchmark calculations. In particular, we compute the circular dichroism of GaN and the rotatory power of trigonal Te and compare our results to those obtained in Ref. [2] at a similar level of theory as ours, as well as previous experimental measurements [3, 4]. We also compute the rotatory power of trigonal Se and discuss our results in light of the substantial effect of local fields recently addressed in Ref. [5] from a density functional perturbation theory standpoint.

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