ELECTRIC, MAGNETIC, AND TOROIDAL POLARIZATIONS IN CRYSTALS

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Multipolar order in bulk crystalline solids is characterized by multipole densities — denoted as *polarizations* in this work — that cannot be cleanly defined using the concepts of classical electromagnetism [1, 2]. We use group theory to overcome this difficulty and present a systematic study of electric, magnetic and toroidal multipolar order in crystalline solids [3]. In particular, we rely entirely on symmetry to extend the notion of bulk dipolarization and magnetization to electric and magnetic multipole densities of higher orders $\ell > 1$. Based on our symmetry analysis, we identify five categories of polarized matter (see Table 1). Each of these categories is characterized by distinct features in the electronic band structure (illustrated in Figure 1). For example, Rashba spin splitting [4] in electropolar bulk materials like wurtzite represents the electric dipolarization in these materials. We also develop a general formalism of indicators for individual multipole densities that provide a physical interpretation and quantification of multipolar order. Our work clarifies the relation between patterns of localized multipoles and macroscopic multipole densities they give rise to. To illustrate the general theory, we discuss its application to polarized variants of hexagonal lonsdaleite and cubic diamond structures. Our systematic approach provides a broader framework for recent efforts to study electric and magnetic multipolar order in solids [5, 6] and lends itself for wider application in the context of complex materials [7, 8].

Table 1: Families of electric, magnetic, and toroidal multipole densities (*polarizations*) of order ℓ permitted by the five inversion goups formed from space inversion i and time inversion θ. Symmetry operations present (absent) are labeled "•" ("∘"). Polarizations that are allowed (forbidden) under an inversion group are likewise labeled"•" ("∘"). We also list the signature ss' for each family of polarizations, with $s = \pm$ ($s' = \pm$) indicating transformation behavior under i (θ). Each inversion group defines a category of polarized matter, as indicated in the last column.

inversion group	symmetry i	θ	$i\theta$	electric ℓ even $++$	electric ℓ odd $-+$	magnetic ℓ even $--$	magnetic ℓ odd $+-$	category of polarized matter
$C_{i\times\theta} = \{e, i, \theta, i\theta\}$	•	•	•	•	∘	∘	∘	parapolar
$C_\theta = \{e, \theta\}$	∘	•	∘	•	•	∘	∘	electropolar
$C_i = \{e, i\}$	•	∘	∘	•	∘	∘	•	magnetopolar
$C_{i\theta} = \{e, i\theta\}$	∘	∘	•	•	∘	•	∘	antimagnetopolar
$C_1 = \{e\}$	∘	∘	∘	•	•	•	•	multipolar

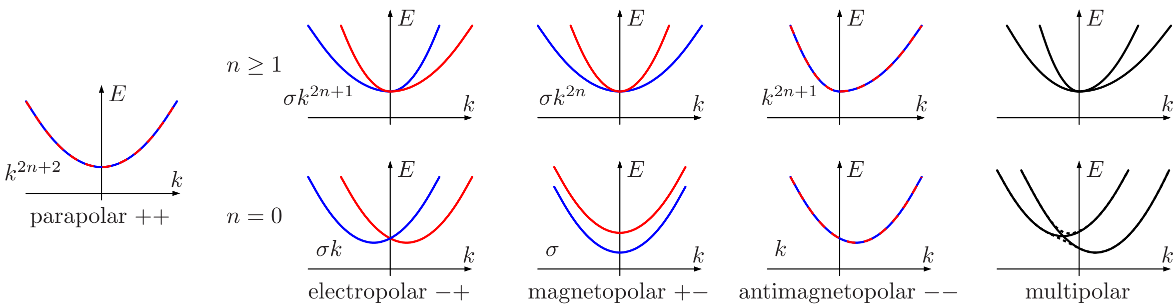

Figure 1: Typical examples for spinful band dispersions $E_\sigma(\mathbf{k})$ associated with the five categories of polarized matter. Different colors represent opposite spin orientations. The symbol n denotes a non-negative integer.

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