THEOS
THEORY AND SIMULATION OF MATERIALS

cecam
Centre Européen de Calcul Atomique et Moléculaire

EPFL
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Axion electrodynamics in condensed matter: Magnetoelectric materials

Professor Raffaele Resta
Dipartimento di Fisica, Universita' di Trieste, and
DEMOCRITOS Simulation Center, CNR-IOM, Trieste

Tuesday Mar 13, 15:00, Room MXC 315

Abstract: The energy density of an electric field **E** is proportional to **E·E**, and that of a magnetic field **B** is proportional to **B·B**. What about an electrodynamics where a further quadratic term **E·B** appears? Such a term, dubbed "axion", has been postulated in high-energy physics, and its consequences investigated. Axion electrodynamics is indeed realized in condensed matter, where the coupling term takes the form **E·H**, provided that the medium breaks both inversion symmetry and time-reversal symmetry. The paradigmatic single-crystal magnetoelectric (ME) is Cr_2O_3, which in fact is non centrosymmetric and antiferromagnetic. In ME materials an electric field induces macroscopic magnetization, and a magnetic field induces electrical polarization. In most materials the effect is very weak; the search for strong MEs is an active area of research.

In ordinary dielectrics the field E is coupled to the electronic polarization as well as to the lattice, via the ionic charges. This has three important consequences: (1) the static dielectric constant (or tensor) ε_0 is different form the electronic one ε_∞ (also called "clamped nuclei" dielectric constant); (2) the phonon spectrum is nonanalytic at short wavevectors; (3) The zone-center phonon frequencies are related to the dielectric constants by the Lyddane-Sachs-Teller (1941) relationship, nowadays in every solid-state-physics textbook. Due to the axion term, both fields **E** and **H** contribute to the coupling on equal footing in MEs, and therefore the points (1-3) above need a complete reformulation; this has been recently achieved [1,2].

Two more specialized topics are possibly discussed: (i) To a first-principle theorist, the macroscopic fields of choice are **E** and **B**, not **H**: they enter e.g. the Kohn-Sham Hamiltonian. The solution of the **H** vs. issue is provided [2]. (ii) A magnetic field does not exert any force on a nucleus at rest: so which is the origin of the magnetic lattice coupling? The answer to this question is provided [2].

[1] R. Resta, Lyddane-Sachs-Teller Relationship in Linear Magnetoelectrics, Phys. Rev. Lett. 106, 047202 (2011).
[2] R. Resta, Zone-Center Dynamical Matrix in Magnetoelectrics, Phys. Rev. B 84, 214428 (2011).