The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

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FIFTH STIG LUNDQVIST CONFERENCE ON THE ADVANCING FRONTIERS OF CONDENSED MATTER PHYSICS
11 - 15 July 2011

ORBITAL MAGNETOELECTRIC EFFECTS AND TOPOLOGICAL INSULATORS

David VANDERBILT
Dept. of Physics, Rutgers University Piscataway, New Jersey, U.S.A.

ABSTRACT:

The concepts of the Berry potential and Berry curvature play an important role in the theories of electric polarization, orbital magnetization, and the anomalous Hall effect. I shall briefly review these topics, and then discuss how these concepts can be applied to develop a theory of the linear orbital magnetoelectric effect in multiferroic insulators. Remarkably, there is a geometric contribution to the magnetoelectric tensor [1-2] that depends on the Berry potential and curvature according to the Chern-Simons three-form, a structure that is more complicated than, but highly analogous to, the Berry-phase polarization expression. For example, this geometric magnetoelectric coupling θ is only well-defined modulo 2π; shifting it by a quantum corresponds to the addition of a a surface layer exhibiting an integer quantum Hall effect, just as shifting P by 2π corresponds to the occupation of an extra surface-state band.

Insulators obeying time-reversal symmetry must either have θ = 0 or π, these being the two values that are mapped into themselves, modulo 2π, by θ → −θ. This provides a topological classification that is equivalent to the division into “normal insulators” and “strong topological insulators” (STI) in 3D [1,2]. The assignment of θ = π to a STI having time-reversal symmetry seems paradoxical, since a sample of such a material cannot show any experimental magnetoelectric effect if time-reversal symmetry is unbroken. This appar- ent paradox can be resolved by considering also the surface contributions, and considering carefully the cases that time-reversal symmetry is, or is not, broken at the surface [3].

The axion contribution to the orbital magnetoelectric tensor is not the only one. Even in the frozen-ion orbital sector, there are additional Kubo-like contributions [4-5]. There are also frozen-ion spin (Zeeman) contributions, as well as lattice-mediated orbital and spin contributions. We have computed all of these contributions for the case of Cr2O3, a well- studied magnetoelectric material.

Finally, I shall present a method for computing the Z2 invariant that is well suited to the complex bandstructures that often emerge from first-principles calculations [6]. The method works regardless of whether inversion symmetry is present, and is efficient and easily automated. Applications to a few normal and strong topological insulators will be presented.

*Collaborators: S. Coh, A.M. Essin, A. Malashavich, J.E. Moore, A.A. Soluyanov, I. Souza, and A.M. Turner.

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