Calculation of the Chern-Simons orbital magnetoelectric coupling

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Recently it was shown[1,2] that the orbital part of the linear magnetoelectric coupling (MEC) in an insulator has a geometric-phase contribution that is isotropic and can be characterized by a coupling θ that is only well-defined modulo 2π. Furthermore, this θ in strong Z_2 topological insulators is unusually large and equals exactly half a quantum ($\theta = \pi$). Experimental observation of this large MEC would require some peculiar breaking of the time-reversal (T) symmetry at the surfaces, but θ might be observed in normal insulators that have T already broken in the bulk. Since there are by now several examples of strong Z_2 topological insulators having $\theta = \pi$, we believe there is no strong reason why θ should necessarily be small in a normal insulator with broken T. For this reason, we have used density-functional theory to calculate θ in various materials including Cr_2O_3, Fe_2TeO_6, $BiFeO_3$, $GdAlO_3$ and magnetically doped Bi_2Se_3. To calculate θ we express it in terms of well localized Wannier functions to ensure smoothness of the gauge.

[1] Xiao-Liang Qi, Taylor L. Hughes, and Shou-Cheng Zhang, Phys. Rev. B **78**, 195424 (2008),

[2] Andrew M. Essin, Joel E. Moore, and David Vanderbilt, Phys. Rev. Lett. **102**, 146805 (2009).