Calculation of the Chern-Simons orbital magnetoelectric coupling

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Recently it was shown\textsuperscript{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 $\theta$ that is only well-defined modulo $2\pi$. Furthermore, this $\theta$ in strong $\mathbb{Z}_2$ 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 $\theta$ might be observed in normal insulators that have $T$ already broken in the bulk. Since there are by now several examples of strong $\mathbb{Z}_2$ topological insulators having $\theta = \pi$, we believe there is no strong reason why $\theta$ should necessarily be small in a normal insulator with broken $T$. For this reason, we have used density-functional theory to calculate $\theta$ in various materials including Cr$_2$O$_3$, Fe$_2$TeO$_6$, BiFeO$_3$, GdAlO$_3$ and magnetically doped Bi$_2$Se$_3$. To calculate $\theta$ we express it in terms of well localized Wannier functions to ensure smoothness of the gauge.
