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Calculation of the axion magnetoelectric coupling SINISA COH, DAVID VANDERBILT, Rutgers University, ANDREI MALASHEVICH, IVO SOUZA, UC Berkeley — Recently it was shown [X.-L. Qi *et al.*, PRB **78**, 195424 (2008); A.M. Essin *et al.*, PRL **102**, 146805 (2009)] that there exists a purely isotropic ("axionic") component θ to the magnetoelectric coupling (MEC). Furthermore, this θ arises only from the electron orbital motion, and in strong Z_2 topological insulators it 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. We first consider Cr_2O_3, a widely studied magnetoelectric material, but we find θ to be very small there. We attribute this to a weak spin-orbit effect in Cr (and to the fact that even a strong spin-orbit effect by itself does not guarantee a large θ). To calculate θ we express it in terms of well localized Wannier functions to ensure smoothness of the gauge and also to allow for decomposition of contributions to θ coming from various electronic bands. The calculation of θ for $BiFeO_3$ and other materials is currently ongoing.

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